A SIMPLE MODEL FOR SIMULATION OF THE FATE OF MINERAL MATTERS IN A COAL FIRED BOILER

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1977

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
the requirements for
the Degree of
MASTER OF SCIENCE
July, 1988

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ABSTRACT

A major problem in the operation of coal fired boilers is the formation of slag and fouling of the boiler tubes. The slagging problem may become detrimental to the operation of the boiler, especially when different coals are blended. The objective of this project was to develop a model to predict the composition of slag or fouling at different locations of a boiler. A simple computer model was developed to predict the rate of deposition and the composition of deposits formed at different locations in a boiler. A multicell, lumped parameter approach was used, assuming that the cells are well mixed and deposition occurs only by condensation of the stable minerals on the boiler tubes. An energy balance was used to calculate the coal flame temperature which is then used to estimate the temperature distribution in the boiler. Chemical equilibrium constants were evaluated to define the stable compounds at different temperatures. The amount of each compound deposited at various locations was determined from the vapor pressure of that compound. Predictions of this model are in general agreement with the power plant data suggesting that the dominant compounds in the high temperature zone are the oxides, and the major compounds in the low temperature zone are the sulfates.

ACKNOWLEDGEMENTS

I wish to express my gratefulness to my major adviser, Dr. Mayis Seapan, who was always available to answer questions and make helpful suggestions as well as providing valuable criticism. I would also like to thank Dr. Arland H. Johannes and Dr. Gray L. Foutch for their valuable comments and discussion as members of my committee.

Special thanks are due to the University Center for Energy Research (UCER) for the financial support I received during the course of my thesis work.

My family deserves deepest appreciation for their constant support and encouragement.

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CHAPTER I

INTRODUCTION

Coal has been the main source of energy for generating electricity in the United States and with the continuous depletion of oil and gas resources, its utilization will be growing more rapidly in the coming century. All types of coal contain significant and variable amounts of largely incombustible inorganic compounds, called "mineral matter" or "ash".

The mineral matter primarily includes clays, shales, pyrite, quartz, calcite and lesser amounts of other materials, depending on the chemical and mineralogical composition. This mineral matter content is typically of the order of ten percent by weight in the United States coals. This mineral matter, which must be carried through the combustion process, can form deposits in the boiler, especially in a pulverized-coal-fired system. A typical 900 MW power plant burning about 400 t/h of a pulverized coal containing 10 percent ash produces about 40 t/h of ash (Raask 1985,a). The mineral matter of coal can form bottom ash, slag, fly ash and some fraction may form deposits on heat transfer surfaces inside the boiler. The presence of ash deposits and fly ash can create the following problems

in a boiler:

1. Reduction of heat transfer
2. Impedance of gas flow
3. Physical damage to boiler tubes
4. Corrosion of boiler tubes
5. Erosion of boiler tubes

These problems can result in reduced generating capacity and maldistribution of flow and temperature, eventually resulting in unscheduled shutdowns.

Ash which deposits on boiler walls in the radiant section of a furnace is generally referred to as slag. Ash deposition in the convective section of the furnace is referred to as fouling. Previously, many investigators have used traditional ASTM techniques to correlate the slagging and fouling potential of different coals(Winegartner, 1974). However, these do not always provide the necessary information that can be used to make predictive judgments with a desired confidence level on mineral matter behavior. Especially, when high temperature data available on mineral matter behavior are limited and the work required to obtain additional data is expensive and time consuming. Thus, it has become more desirable to develop suitable models of high temperature behavior of the mineral matter to avoid the time and cost involved in acquiring additional information which are needed for rapid estimation of fuel properties and for continual operation of a boiler with new fuels which have different mineral matter contents.

The process of ash deposit formation is quite complicated. A complete understanding of this process requires a thorough knowledge of fundamental data on chemical composition and distribution of mineral matter in coal, transformations and reactions of the mineral matter in the flame, ash transport mechanisms, initial adhension of ash particles to heat transfer surfaces and subsequently to each other to form a deposit, and further interactions of deposited ash to form a strong deposit. All of these physical and chemical changes during deposit formation are not only coal related but also strongly dependent on the boiler configuration and operational conditions. As a consequence, a precise and quantitative knowledge of the ash deposit formation mechanism has not yet been obtained.

The principal objective of this study is to develop a suitable computer program which can simply and easily determine the composition of the ash deposited at different locations in a combustion chamber by using the regular coal analysis and a few operational parameters. This program is designed to run on IBM compatible Personal Computers, which are easy to use and widely available.

Chemical equilibrium constants are evaluated and used to define the stable ash compounds at different temperatures. A typical temperature profile of a utility boiler is chosen to determine the formation environment of these compounds. Coal flame temperature is calculated to adjust the temperature profiles when different coals are

burned. The amounts of the vapor species are determined by the vapor pressures of the compounds and the distribution of the ash deposits is also determined.

This program is ready for use in an operating power plant. It provides for a rapid estimation of the rate and composition of minerals deposited on the boiler walls. When a change in the coal supplied to an existing boiler is being considered, numerous operating parameters can be simulated through this program to aid in deciding operating strategies that will permit continous operation.

This program can also be used to determine flue gas composition, adiabatic flame temperature, composition and location of deposits, as well as accumulation rates for laboratory scale furnaces (Wang, 1988), if furnace dimension and temperature profile are specified. The results of this program will provide a basis for comparison between theoretical predictions and experimental data, especially at high temperatures.

CHAPTER II

BASICS OF SLAGGING AND FOULING

The coal ash deposition process involves numerous aspects of coal combustion and mineral transformation. The following factors are important in the formation of ash deposits:

1. Boiler configuration and operating conditions
2. Mineral matter characteristics of coal
3. Chemical and physical transformation
4. Ash deposit formation mechanism

The literature review will also focus on these subjects.

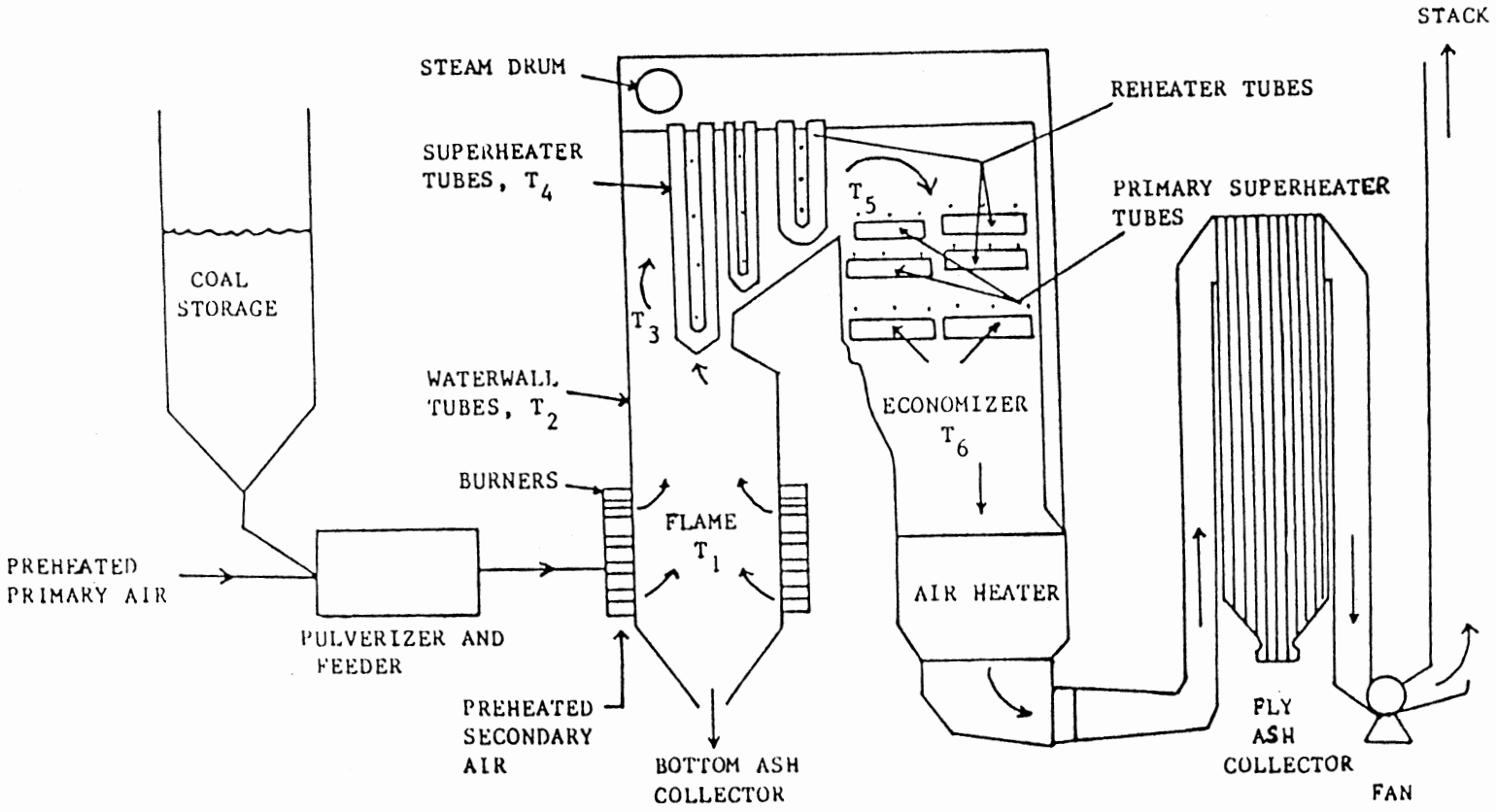
Boiler Configuration and Operating Conditions

A Radiant boiler is often used in utility stations and large industrial plants. The Radiant boiler derives its name from the fact that the transfer of heat is largely by radiation. This boiler is a high-temperature, high-capacity drum type boiler. Boiler convection surface is usually small in these units. It has a nominal output of 1,750,000 lbs/h steam for continuous operation (Bobcock & Wilcox, 1975). The system incorporates the following essential features: coal storage and pulverization, coal and air supply to the burner, ignition, combustion and radiant zones

of heat transfer surfaces in the furnace (waterwall, radiant superheater and reheater tubes), bottom ash removal equipment, on-line tube cleaning facilities (soot blower), steam drum, superheater and reheater tube banks for convective heat transfer, economizer, air heater, fly ash removal equipment, fans, and stack. Figure 1 is a schematic configuration of a typical radiant boiler for pulverized coal.

The pulverized coal and primary air mixture are injected into the furnace via burners, where mixing with the secondary air occurs. The coal particles are heated at 10^5 to 10^6 ^{0}C/s in the flame zone where a loss of moisture followed by the evolution of volatiles occur. As the devolatilization is nearly completed, heterogeneous char combustion dominates the burning of the residual char until the particle is completely burned. Efficient mixing of the burning pulverized coal particles and the combustion air is essential. Particles should have sufficient residence time in the high temperature zone to burn completely.

Temperature in the radiant section may be as high as 1800^0C depending on the coal and process conditions. The heat released in the combustion chamber is either absorbed by the furnace wall tubes or is passed out by the heat content of the flue gas and fly ash. The metal temperature of the waterwall tubes is maintained at about 400^0 C to 450^0 C by water circulating within the tube. The water and steam mixture in the waterwall tubes passes through the riser



T1 = 1500-1700^{O}C; T2 = 400-450^{O}C; T3 = 1200-1400^{O}C;
T4 = 600-650^{O}C; T5 = 1000-1200^{O}C; T6 = 800^{O}C.

Figure 1. Outline of a Typical Radiant Boiler for Pulverize Coal

tubes into the steam drum where the steam is separated from the mixture and passes to superheater tubes. The flue gases (1100 - 1400^{0} C) contact a bank of superheater tubes which further heat the steam before it enters the high-pressure turbines. The exhaust steam from the high-pressure turbines is then returned to the reheater tubes and transported to the low-pressure turbines to increase boiler efficiency. The metal temperature of superheater and reheater tubes may be maintained as high as 650^{0} C, thus high temperature is required to superheat the steam. The steam is condensed after the turbine and this water is transported back to the economizer which removes heat from the flue gases at about 800^{0} C and then recycles to the furnace as the boiler feed water. The flue gases from the economizer enter the air heater where the final heat removal occurs. The air heater has two functions: it cools the flue gases before they pass to the atmosphere and at the same time it raises the temperature of the incoming air to the combustor thereby increasing the efficiency.

Mineral Matter Characteristics

The physical and chemical properties of ash formed from coal combustion are important in determining the potential of a coal to form deposits in boilers. Therefore, it is important to consider the composition and mode of occurrence of the inorganic constituents in coal. Mineral matter is now commonly determined by low-temperature ashing

(Gluskoter, 1965; Frazer and Belcher, 1973; Miller et al., 1979). In addition to the fact that minerals are not altered much by this ashing technique, its main advantage is that the residue can also be a suitable sample for other techniques of mineral identification and analysis. Modern methods of analysis of the minerals in coal are summarized and discussed in detail by Russel and Rimmer (1979) and Gluskoter et al. (1981). The minerals that frequently occur in coals are listed in Table I. Falcone and Schober (1986) applied low temperature ashing (LTA), ASTM, and high temperature ashing (HTA), conducted at 125^{0} C, 750^{0} C and 1000^{0} C respectively, and used XRD to identify the mineral mixtures which are shown in Table II. They concluded that the mineralogies of the raw coals studied do not vary a great deal. Quartz, kaolinite, pyrite and bassanite are found in abundance in each LTA sample. Greater differences between samples are apparent at higher temperatures, because complex aluminosilicates predominate. Some researchers proposed that during combustion quartz and aluminosilicates will react with the volatilized sodium or calcium to form sodium silicates or complex sodium aluminosilicates (Johnson and Litter, 1963; Morgan et al., 1981). Johannes (1977) discussed LTA/HTA ratio for many coals. For bituminous coals, the LTA/HTA ratio is 1.3 to 1.5 and for lignite this ratio will increase.

Pedia (1974,a) proposed that the decrease of mineral matter content in ASTM ash was because of decomposition and

TABLE I

MINERAL MATTERS IN COALS

Mineral	Formular	Usual Proportions
Shale group	$(K,Na,H_3O_3,Ca)_2(Al,Mg,Fe,Ti)_4(Al,Si)_8O_{20}(OH,F)_4$	
Clay group (Kaolinite)	$Al_2O_3 \cdot 2SiO_2 \cdot xH_2O$	50- 90 %
Sulfur group	Fe_2S, $FeSO_4$, Na_2SO_4	Iorn: 0- 20 % Sodium and Potassium: 0- 4 % Sulfur: 0.5- 10 %
Carbonate group	$CaCO_3$, $MgCO_3$	Calcium: 0- 20 % Magnesium: 0- 8 %
Associated minerals		General elements: Sodium and Potassium: 0- 4% Titanium : 0- 2% P,Ni,B,Zr: < 1%
Quartz	SiO_2	
Feldspar	$(K,Na)_2O \cdot Al_2O_3 \cdot 6SiO_2$	
Garnet	$3CaO \cdot Al_2O_3 \cdot 3SiO_2$	
Hornblende	$CaO \cdot 3FeO \cdot 3SiO_2$	
Gypsum	$CaSO_4 \cdot 2H_2O$	
Apatite	$9CaO \cdot 3P_2O_5 \cdot CaF_2$	
Zicron	$ZrSiO_4$	
Epidote	$4CaO \cdot 3Al_2O_3 \cdot 6SiO_2 \cdot H_2O$	
Biotite	$K_2O \cdot MgO \cdot Al_2O_3 \cdot 3SiO_2 \cdot H_2O$	
Augite	$CaO \cdot MgO \cdot 2SiO_2$	
Prochlorite	$2FeO \cdot 2MgO \cdot Al_2O_3 \cdot 2SiO_2 \cdot 2H_2O$	
Diaspore	$Al_2O_3 \cdot H_2O$	
Lepidocrocite	$Fe_2O_3 \cdot H_2O$	
Magnetite	Fe_3O_4	
Kyanite	$Al_2O_3 \cdot SiO_2$	
Staurolite	$2FeO \cdot 5Al_2O_3 \cdot 4SiO_2 \cdot H_2O$	
Topaz	$(Al,F)_2\ SiO_4$	
Tourmaline	$MgAl_3(BOH)_2Si_4O_{19}$	
Hematite	Fe_2O_3	
Penninite	$5MgO \cdot Al_2O_3 \cdot 3SiO_2 \cdot 2H_2O$	

(Godridge and Read, 1976)

TABLE II

MINERALOGOCAL COMPOSITION OF ASH SAMPLES
DETERMINED BY XRD

Coal type	LTA(125^{O}C)	ASTM(750^{O}C)	HTA(1000^{O}C)
Absaloka	Quartz Pyrite Kaolinite Plagioclase Bassanite	Quartz Andydrite Hematite	Anhydrite Magnetite Hematite Quatz Melilite Plagioclase Nepheline
Beulah- Low Na	Quartz Pyrite Kaolinite Bassanite	Quartz Hematite Magnetite Anhydrite	Anhydrite Pyroxene Magnetite Hauyne Hematite Quartz
Beulah- High Na	Quartz Bassanite Kaolinite Pyrite	Anhydrite Hematite Magnetite Quartz Melilite Hauyne	Anhydrite Melilite Magnetite Hematite Hauyne Quartz Corundum
Center	Quartz Bassanite Pyrite Kaolinite	Anhydrite Hematite Quartz	Anhydrite Hauyne Pyroxene Melilite Hematite Quartz
Choctaw	Quartz Pyrite Kaolinite Bassanite Plagioclase	Anhydrite Quartz Hematite Magnetite Plagioclase Pyroxene	Anhydrite Hematite Quartz Magnetite Plagioclase

TABLE II (Continued)

Coal type	LTA(125^{O}C)	ASTM(750^{O}C)	HTA(1000^{O}C)
Falkirk	Quartz Kaolinite Pyrite	Anhydrite Quartz Hematite Magnetite Melilite	Anhydrite Quartz Melilite Hematite Magnetite Hauyne
Gascoyne Blue-High Na	Quartz Kaolinite Pyrite Calcite Sodium Sulfate	Anhydrite Quartz Hematite Magnetite Nosean Melilite	Anhydrite Melilite Hauyne Quartz
Gascoyne Read-Low Na	Quartz Kaolinite Pyrite	Anhydrite Quartz Hematite Magnetite	Anhydrite Quartz Hauyne Pyroxene Hematite
Indian Head-High Na	Quartz Pyrite Kaolinite Bassanite	Anhydrite Quartz Hematite Nosean Melilite Hauyne Sodium Sulfate	Melilite Hematite Anhydrite Hauyne Magnetite Pyroxene
Pike	Quartz Kaolinite Pyrite	Anhydrite Quartz Pyrite	Anhydrite Hematite Melilite Anorthite Quartz
Velva	Quartz Kaolinite Pyrite Bassanite	Anhydrite Quartz CaO	Anhydrite Gehlenite Quartz MgO Hauyne

(Falcone and Schobert, 1986)

volatilization losses during ashing process. The losses are mainly due to the partial or complete loss of water of kaolinite and illite, conversion of pyrite to ferric oxide and dissociation of carbonates and sulfates to metal oxides with the release of CO_2 and SO_2. He also reported a relation between the mineral matter and ash content based on the proposed decomposition scheme and a material balance.

$$\text{Mineral matter} = \text{ash} + 0.625S_{\text{pyrite(coal)}} + 0.833S_{\text{sulf(coal)}}(1 - \text{ash}/100.0) + (\text{ash}/100)(0.162(SiO_2 + Al_2O_3)_{\text{ash}} + 0.79CaO_{\text{ash}} + 1.1MgO_{\text{ash}})$$

The silicate minerals, kaolinite and aluminosilicate species together with quartz constitute the bulk of mineral matter in most coals. The silica (SiO_2) and alumina (Al_2O_3) as determined by ASTM analysis are present in alumino-silicates on an average weight ratio of 1.5 to 1.0 as reported by Dixon et al. (1970). Based on these, Raask(1985, b) proposed methods to quantitatively determine the approximate amounts of different silicate species of bituminous coal mineral matter from ash analysis. The excess of silicate represents the amount of quartz in coal mineral matter:

$$(SiO_2)_q = (SiO_2)_t - 1.5(Al_2O_3)$$

where $(SiO_2)_q$, $(SiO_2)_t$ and (Al_2O_3) denote the quartz, total silica and alumina contents of ash respectively. The

potassium alumino-silicate content of coal mineral matter (K_{Al-Si}) by weight percent is:

$$K_{Al-Si} = \frac{K_2O}{0.11} = 9.1K_2O$$

where K_2O denotes the potassium oxide content of ash. Since the total amount of silicate mineral equals approximately the sum of SiO_2, Al_2O_3 and K_2O in ash, an estimate of kaolinite is given by:

$$\text{kaolinite} = (SiO_2)_t + Al_2O_3 + K_2O - (SiO_2)_q - K_{Al-Si}.$$

Table III gives the SiO_2, Al_2O_3 and K_2O contents of some U.S. and British bituminous coal ashes and uses this estimation technique to calculate the approximate amounts of quartz, potassium alumino-silicate and kaolinite in the mineral matter. From this table it is found that silicate minerals usually account for between 60 - 90 percent of the total minerals in coal.

Chemical and Physical Transformations

The mineral matter undergoes two different types of transformations in a pulverized coal combustion process. These are the chemical transformation and the physical transformation, which will be discussed here.

Chemical Transformation

The identification of coal minerals and their chemical

TABLE III

ESTIMATED AMOUNTS OF SILICATE SPECIES IN BITUMINOUS COAL MINERAL MATTERS

Coal Type		Ash Constituents (Weight % of Ash)			Mineral Species (Weight %)		
		SiO_2	Al_2O_3	K_2O	Quartz	Alumino-Silicates	Kaolinite
Low SiO_2	GB	31.1	18.1	1.2	3.9	10.9	26.2
	US	29.2	14.2	1.5	7.9	13.6	23.6
Med. SiO_2	GB	46.5	22.8	2.8	12.3	25.5	34.3
	US	46.6	27.8	1.1	4.9	10.0	60.6
High SiO_2	GB	55.5	30.0	2.7	10.5	24.5	53.2
	US	56.5	32.2	2.6	8.0	23.6	59.7
Jacobs Ranch*		46.4	13.8	1.4	25.7	13.2	22.7
Clovis Point*		50.2	13.6	1.5	29.9	12.5	22.9

* used the same estimation technique to calculate two Wyoming coals

(Raask, 1985, b)

transformation at high temperatures have been studied by various investigators (Selvig and Gibson, 1956; Ramsden, 1969; Halstead and Raask, 1969; O'Gorman and Walker, 1971; Boow, 1972; Augustyn et al., 1976). Table IV indicates the general changes of mineral matter found at various temperature levels (Gluskoter and Mitchell, 1976). Most of the high temperature transformation works have consisted of differential thermal analysis studies and X-ray diffraction studies in which the coal minerals were heated slowly. The transformations observed in these works are apparently slow processes with respect to chemical kinetics. These studies do not simulate the rapid heating conditions in pulverized coal combustion (10^5 - 10^6 ^{0}C/s). Therefore, it is not clear whether they correspond to the more rapid transformations occurring during actual combustion processes.

Pedia (1976,b) simulated the actual combustion conditions in a free fall furnace from 777^{0}C to 1557^{0}C and concluded that the chemical transformations of the principal mineral constituents are as given in Table V. Compared with ASTM ash, the weight loss of ash increased with the increase of furnace temperature. The weight loss was attributed to the thermal decomposition of kaolinite, carbonates and the oxidation of pyrites. For higher temperatures, additional losses were observed which were mainly by decomposition of $CaSO_4$ and the vaporization of silica and other oxides. Falcone and Schobert (1986) modeled mixtures of the major

TABLE IV

GENERAL CHANGES OF MINERAL MATTERS AT VARIOUS TEMPERATURES

(4 5 6 7 8 9 10 11 12 13 14)*100^{O}C
←---------- Quartz SiO_2 ----------→ ←- amorphous -→
←kaolinite→ ←-metakaolinite→ ←----------mullite----------→ $Al_2O_3 \cdot 2SiO_2$ $2H_2O$(clay)
←-illite--→ ←----------amorphous----------→ $K(Si)Al_2O_{10}(OH)$
←-pyrite--→ ←----------hematite----------→ FeS_2 Fe_2O_3
←-calcite-→ ←---------anorthite---------→ $CaCO_3$ lime and anhydrite CaO
←--gypsum-→ ←----------anhydrite----------→ $CaSO_4 \cdot 2H_2O$ $CaSO_4$

(Gluskoter and Mitchell, 1976)

TABLE V

PRINCIPAL REACTIONS OF MINERAL MATTERS
IN OXIDIZING ATMOSPHERE

Species	Reaction	Apporximate Reaction Temperature, ^{0}C
Kaolinite $Al_2Si_2O_5(OH)_4$	$Al_2Si_2O_5(OH)_4$ $\rightarrow Al_2O_3\ 2SiO_2+2H_2O$ $\rightarrow Al_2O_3+2SiO_2$	550 - 600
Pyrite FeS_2	$2FeS_2+3.5O_2$ $\rightarrow Fe_2O_3+4SO_2$	500
Sulphate		
$CaSO_4$	$CaSO_4 \rightarrow CaO+SO_3$	1450
$MgSO_4$	$MgSO_4 \rightarrow MgO+SO_3$	1000
$Fe_2(SO_4)_3$	$Fe_2(SO_4)_3$ $\rightarrow Fe_2O_3+3SO_3$	600
Carbonates		
$CaCO_3$	$CaCO_3 \rightarrow CaO+CO_2$	710 - 950
$CaMg(CO_3)_2$	$CaMg(CO_3)_2$ $\rightarrow CaO+MgO+2CO_2$	740-800

(Pedia, 1976, b)

mineral matter which are given in Table VI. Greater differences between samples are apparent at higher temperatures, where complex aluminosilicates predominate.

Physical Transformations

The physical transformations that mineral matters undergo include fusion, agglomeration, vaporization and formation of cenospheres (Sarofim et al., 1977).

Frenkel(1945) has shown that the fusion time, t, of transformation of an irregularly shaped particle to a sphere is given approximately by:

$$r = r_0 e^{-t/z}$$

r = the distance of a point on the original surface from the center of a sphere of equivalent volume having radius r_0

where $z = 4\pi\eta/\gamma$.

η = viscosity.

γ = surface tension.

If the value of surface tension and time of exposure to high temperature is known, the viscosity at which the irregular shape particle transforms to sphere can be calculated. Raask(1986,c) concluded that the small irregularly shaped particles should transform to sphere in a coal flame because the viscosity of silicate glassy material is several orders higher than that required for bulk flow under gravity which is about 25 Nsm^{-2}.

TABLE VI

SYNTHETIC COMPOUND MIXTURES AND TRANSFORMATIONS OCCURRING DURING HEATING

Compound Mixtures	Molar Ratios	Temp °C	Analyzed Minerals	Processes
$Ca(C_2H_3O_2)_2$ + FeS_2	2:1	750	Anhydrite($CaSO_4$) + Magnetite(Fe_2O_3)	Oxidation
		1000	Anhydrite($CaSO_4$) + Magnetite(Fe_3O_4) + Hematite(Fe_2O_3)	Oxidation
$CaCO_3$ + FeS_2	1:2	750	Anhydrite($CaSO_4$) + Calcite($CaCO_3$) + Hematite(Fe_2O_3)	Oxidation
		1000	Anhydrite($CaSO_4$) + Hematite(Fe_2O_3) + Magnetite(Fe_3O_4) + CaO	Oxidation
$Ca(C_2H_3O_2)_2$ + $Al_2Si_2O_5(OH)_4$	1:1	750	Amorphous + CaO	Oxidation Dehydration
		1000	Gehlenite ($Ca_2Al_2SiO_7$)	Reordered
$NaC_2H_3O_2$ + $Al_2Si_2O_5(OH)_4$	1:1	750	Amorphous + Carnegieite ($NaAlSiO_4$)	Dehydration Reordered
		1000	Nepheline ($NaAlSiO_4$)	
$CaCO_3$ + $Al_2Si_2O_5(OH)_4$	2.5:1	750	Calcite($CaCO_3$) + Amorphous phase	Dehydration Collapse
		1000	Gehlenite ($Ca_2Al_2Si_2O_7$) + CaO + Mullite	Reordered
Na_2SO_4 + $Al_2Si_2O_5(OH)_4$	1:1	750	Na_2SO_4 + Amorphous	Dehydration
		1000	Nepheline ($NaAlSiO_4$)	Reordered

TABLE VI (Continued)

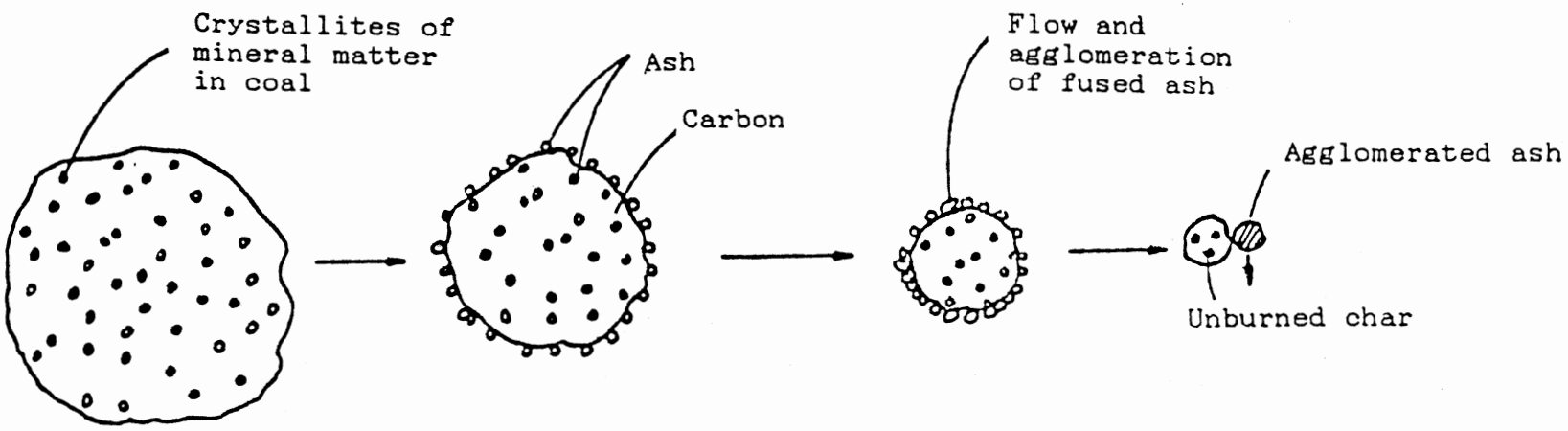
Compound Mixtures	Molar Ratios	Temp ^{O}C	Analyzed Minerals	Processes
$Al_2Si_2O_5(OH)_4$ + Na_2SO_4 + $Ca(C_2H_3O_2)_2$	1:1:1	750	Na_2SO_4 + Amorphous	Dehydration
		1000	Gehlenite ($Ca_2Al_2SiO_7$) + Nepheline ($NaAlSi_4$) + Hauyne $(Na,Ca)_{6-8}(AlSiO_4)(SO_4)_{1-2}$	Reordered
$Al_2Si_2O_5(OH)_4$ + $NaC_2H_3O_2$ + $Ca(C_2H_3O_2)_2$ + FeS_2	1:1:1:1	750	Magnetite(Fe_2O_3) + Anhydrite($CaSO_4$	Dehydration Oxidation
		1000	Hauyne + Hematite (Fe_2O_3)+ Magnetite (Fe_3O_4)+ Anhydrite ($CaSO_4$)+ Gehlenite ($Ca_2Al_2SiO_7$)	Reordered Oxidation
$Al_2Si_2O_5(OH)_4$ + SiO_2 + $NaC_2H_3O_2$ + $Ca(C_2H_3O_2)_2$ + FeS2	1:2:1:1:1	750	Quartz(SiO_2) + Anhydrite($CaSO_4$) + Hematite(Fe_2O_3)	Dehydration Oxidation
		1000	Quartz(SiO_2) + Anhydrite($CaSO_4$) + Hauyne + Hematite (Fe_2O_3) + Magnetite (Fe_3O_4)	Reordered Oxidation

(Falcone and Schobert, 1986)

The agglomeration of mineral matter in coal has been studied by several investigators (Paulson and Ramsden, 1970; Ramsden, 1969; Lightman and Street, 1968; Street et al., 1969). As a coal particle burns, the combustion front approaches and passes the fused ash droplet, the ash particle may separate or continue to attach to the shrinking carbon. Whether the ash particles will detach from the surface of the char particle or not depends upon the balance between the gravitational force and the surface tension. When the carbon is completely consumed all the droplets coalesce into a single droplet. This ash droplet will eventually solidify. This mechanism is for complete agglomeration of all mineral particles within a coal particle which would give one ash particle per coal particle. Figure 2 (Pedia, 1976,c) demonstrates this mechanism.

Actually, fragmentation of a coal particle may take place during combustion. Therefore, agglomeration of mineral particles will only partially occur, and the number of ash particles per coal particle is determined by the fragmentation of the coal particles. Sarofim et al. (1977) reported that from the size distribution of the particles and their mean density, it is estimated that about 3 ash particles per coal particle are formed for the lignite and 5 ash particles per coal particle are formed for bituminous coal.

As a coal particle is heated in an oxidizing



(Pedia, 1976,c)

Figure 2. Ash Agglomeration Mechanism For a Shrinking Core Coal

environment, the mineral matter proceeds fusion, agglomeration, and fragmentation. As the temperature rises further, ash heating, melting and vaporization proceed simultaneously. For an magnetohydrodynamic (MHD) combustor with small residence time (50 ms) and high temperatures (2700 K), complete vaporization of SiO_2 is possible and other metal oxides, such as Al_2O_3, MgO, CaO, would vaporize partially. Therefore, estimation of the amounts and the composition of vaporized ash is very important in predicting the slag formation.

Another phenomenon in physical transformations is formation of cenosphere. Cenospheres are caused by the internal evolution of gases which can result in expansion, and formation of large hollow ash particles. The formation and size of cenospheres are controlled by the viscosity and surface tension of the fused ash, the rate of gas evolution, and the rate of diffusion of gas through the melt. A theoretical study was performed by Sarofim et al.(1977). They concluded that below 727 ^{0}C cenospheres would not be formed because residence times are too small. Above 1327 ^{0}C, the cenospheres have ample time to form and consequently collapse. An optimum temperature of cenosphere formation is between 927 ^{0}C and 1127 ^{0}C.

Lauf (1981) reported ashes with high amounts of Fe_2O_3 (above 20 percent) do not produce significant amounts of cenospheres. This may be because the iron-rich ashes have a low viscosity and the gas evolution is too rapid for the

formation of stable cenospheres.

Raask (1985,d) mentioned the longer the residence time the higher the formation of cenospheres. Therefore, the amount of cenospheres formed in small size pulverized-coal-fired boilers are higher than those produced by a large size pulverized-coal-fired boilers.

Ash Deposits Formation Mechanism

The principles of ash deposition in coal fired boilers are similar to those in gas turbines which have been reviewed by Garner and Seapan (1984). However, the presence of high concentrations of low volatile minerals in coal fired boilers makes the analysis of the problem more complicated than that in gas turbines.

After leaving the combustion zone, the vaporized minerals condense on the boiler tubes. Figure 3 shows this transformation (Brown, 1966). From this simple picture it can be observed that the important parameters in the formation of ash deposits are residence time, temperature, and pressure history and the composition and type of the minerals. The time and temperature history are kinetic factors and can be determined from the configuration and operation of the combustion reactor. While the pressure history is a thermodynamic factor and can be approached from the vapor pressure of the mineral species. Based on this picture, by maintaining the temperature above the condensation point of the species one can control the vapor

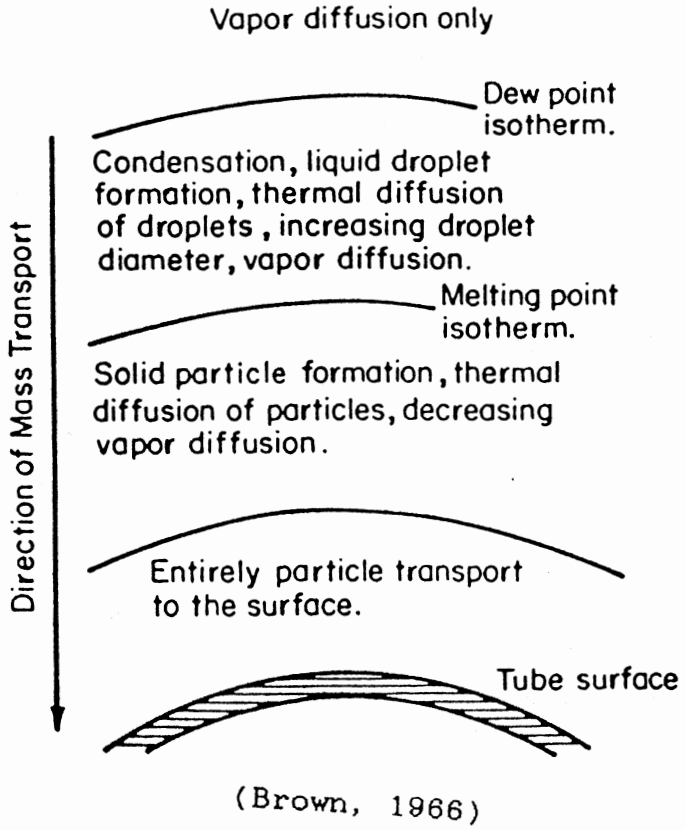


Figure 3. Mechanism of Deposition by Vapor Diffusion

phase deposition. Therefore, flue gas temperatures are usually kept above 1100 ^{0} C before reaching the superheater tubes.

In parallel to the condensation of mineral vapors, the residual combustion particles and fly ash particles also deposit on the boiler tubes. The formation mechanism of an ash deposit on heat transfer surfaces in pulverized coal fired boilers can be explained by the following sequence:

1. Fly ash formation and transpiration towards the heat transfer tubes;

2. Initial adhension of ash particles onto the heat transfer tubes and further deposit build up (the sticking process);

3. Interactions between the deposited ash particles form a strong deposit (the sintering process).

In the first stage, the transport of ash particles from the high temperature flue gas to the boiler tubes takes place by initial impaction or diffusion. This mechanism depends on the size and mass of ash particles, velocity of the particles and temperature of the heating surfaces (France et al.,1984). During impaction, particles above 10 micrometers in diameter in the convetoinal boilers have kinetic energy high enough to be dispersed, resulting in their rebound into the flue gas (Raask, 1986, e). Vapor diffusion and condensation occur when the surface temperature is cool enough to produce a local saturation of vapors. In general, the vapor diffusion and condensation

processes are more likely to form "sticky" surfaces than the inertial impaction of particles, since the condensates are probably liquid.

In the second stage, deposits form because retention occurs on surface contact. This retention depends on three factors: the inherent surface roughness of the tube, the electrostatic attraction between the fly ash and the tube surface, and the presence of sticking compounds on the tube surface. The first two factors allow less fusible fly ash to remain in close contact on the tube surface for sufficient time to form ash deposits with other condensed compounds. The sticky process is due to vapors that condense on the tubes to form a sticking coating which then collects less fusible fly ash particles. Austin et al. (1985) developed an apparatus to study the sticking or adhesion behavior of slag. Three points were stressed:

1. higher substrate temperature results in stronger adhesion,

2. higher flue gas temperature causes more particles to stick,

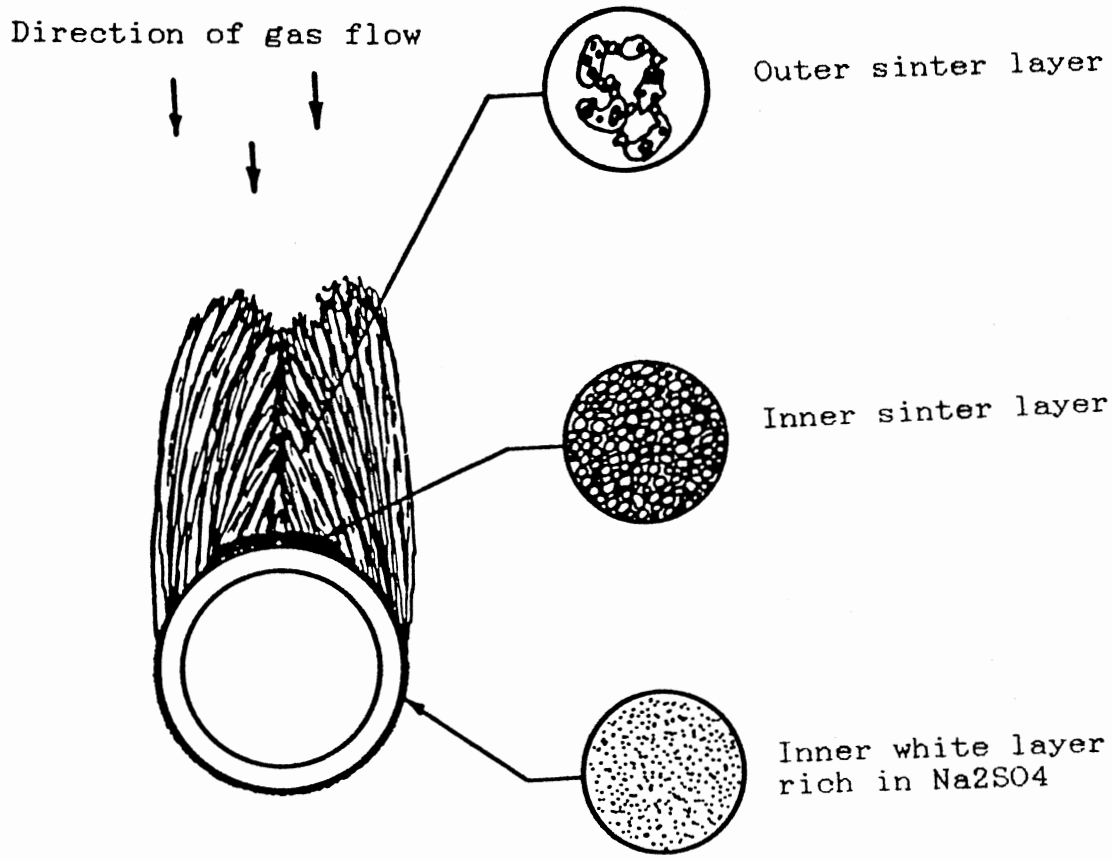
3. ash particles with higher melting points are more likely to form supercooled glasses.

The third stage is the sintering process. The alkali metals dissolved in flame-heated silicate-ash particles have a low vapor pressure, but they can significantly reduce the viscosity and increase the rate of sintering (Boow, 1972). Therefore, sintering by viscous flow is a dominant role in

the formation of deposits in coal fired boilers. In most coal deposits, the volatile sodium plays an important role in initiating the sintering but the subsequent deposit formation depends largely on the presence of calcium and iron oxides. The rate of sintering is proportional to the surface tension of the glassy phase and inversely proportional to the particle size and the viscosity. Rapid sintering occurs from 1127^{0}C to 1277^{0}C (Raask, 1985,f). This is due to the presence of a liquid phase or molten layer on the surface of ash particles.

Figure 4 shows a simple and typical structure of deposits formed from burning coal (Sondreal et al., 1977). Other graphical demonstrations concerning the deposit formation mechanisms can be found in France et al. (1984), Quann and Sarofim (1982) and Flagan (1977).

Viscosity is an important rate-controlling parameter which determines the rates of coalescence to form the boiler deposits. The viscosity-temperature relationship of an ash is often used to predict the fluidity of the coal ash deposition. The temperature of critical viscosity (T_{cv}) is the temperature at which the viscosity properties of the molten slag change from a Newtonian fluid to a Bingham fluid. This is also denoted as the temperature at which solid phases start to crystallize from their melting states. A combination of temperature required for a given viscosity and T_{cv} can be used to estimate the extent of slag build up on the water wall tubes in a fire box.



(Sondreal et al., 1977)

Figure 4. Typical Structure of Deposits Formed from Burning Coal

CHAPTER III

MODELING OF ASH DEPOSITION

The pulverized-coal-fired boilers are the principal generating units for converting coal to electricity. The growing capacity of these boiler units has made it vitally important to rapidly estimate the fuel properties and to decide the operating strategies. As mentioned earlier, the high temperature data are hard to find and expensive to obtain, therefore, a model can be a valuable means in order to quickly and quantitatively provide the operating strategies.

In chapter II a comprehensive discussion of the mechanisms involved in the formation of ash deposits on the boiler tubes of coal fired boilers was presented. Development of a model considering all mechanisms will be very involved. The two classes of mechanisms responsible for conveying mineral matter to the tube surfaces are condensation of mineral vapors and deposition of particles. The mass transport of mineral vapors and their condensation on the boiler tubes may form a sticky coating which can facilitate the collection of particles from combustion gases. Meanwhile the mineral vapors can condense in the gas phase to form suspended particles which can deposit on the

boiler walls by different mechanisms. Condensation of vapors is considered as the major slagging mechanism. Therefore in this project, as a first step in simulating mineral matter depositions on boiler walls, only condensation will be considered. For condensation of vapors, the most important parameter is the temperature distribution in the boiler. There are many important parameters that can influence the temperature distribution in a boiler, for example, fuel composition, furnace geometry, combustion conditions, excess air, and ash content. To simplify this case, a typical temperature profile was chosen. Since different coals release different amounts of energy, their temperature profiles are estimated by modifying the typical temperature profile using the adiabatic flame temperature of the coal of interest. Since the mineralogies of the raw coals do not vary too much, after the combustion process the mineral matters will tend to form similar stable compounds. These compounds will then form deposits based on their vapor pressures. To determine the distribution of the deposition, a multicell, lumped parameter approach is used. The combustor is divided into a number of well-mixed cells. Each cell is assumed to be uniform in its properties and has only one constant temperature. The vapor distribution of the stable compound can be determined from its vapor pressure within each cell. If deposition occurs only by condensation, the distribution of the solid deposit and the residual vapor in each cell can

be determined by a mass balance. Figure 5 shows a schematic diagram of this model which divides a boiler into N equal stages with each stage being 10 feet in height. In each stage, the mineral matter vapors from the lower stage condense partially, and form deposits on the wall while the rest of the vapor continues to move upward to the next stage. The major assumptions of this model are as follows:

1. Mineral matter deposition occurs only by condensation of the stable minerals on the boiler tubes.

2. The boiler is at steady state.

3. The combustor is perfectly mixed and the pulverized coal burns immediately in the boiler.

4. The wall temperature at any location is assumed to remain constant and not change with accumulation of slag on the wall.

5. The vapor phase of the mineral compound follows the ideal gas law.

The conceptual model will include the following steps:

1. Calculation of the coal flame temperature.

2. Qualitative and quantitative determination of the possible deposits.

3. Estimation of the temperature profile to account for the operating conditions.

4. Suitable vapor pressure equations to account for the vapor behavior of the ash deposits.

5. Calculation of the stable deposit distribution at different heights.

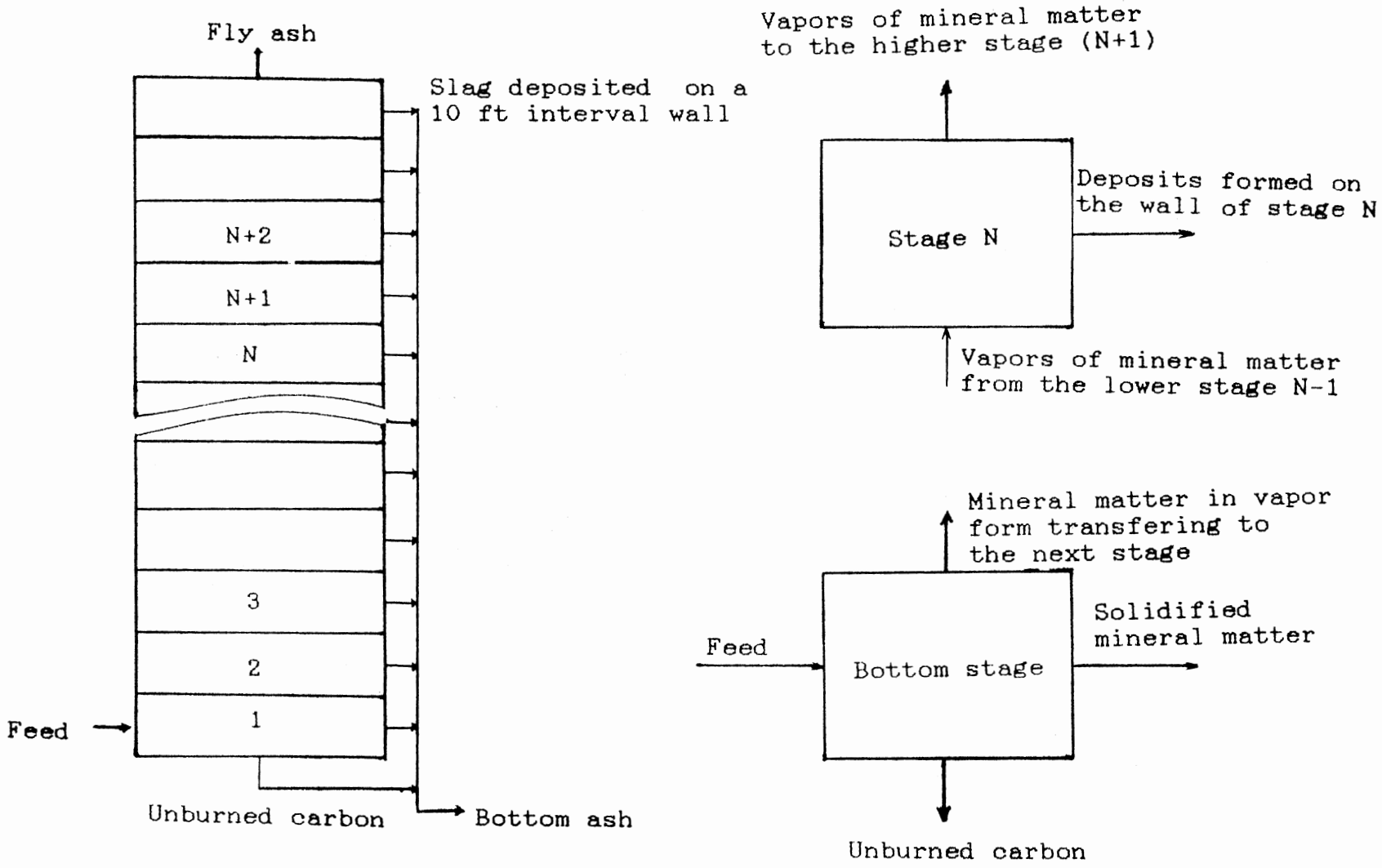


Figure 5. Schematic Diagram in Modeling Ash Deposition

Adiabatic Flame Temperature

The adiabatic flame temperature is the maximum theoretical temperature which can be reached by the products of combustion of a specific fuel with air assuming no loss of heat to the surrounding and no change of kinetic or potential energy until combustion is completed. This is the maximum temperature that can be achieved for a given fuel because any incomplete combustion would tend to lower the temperature of the products. The heat of combustion of the fuel is the major factor in the flame temperature, but changing the temperature of the air or the fuel will also change the flame temperature.

To calculate this temperature, the following assumptions are made:

. There is no conversion of thermal energy to other forms of energy.

. The system is at a constant pressure of 1 atm.

. The reference temperature is $25^{O}C$.

. Instantaneous and perfect mixing of fuel.

In this calculation the input information comes mostly from the regular coal analysis which includes the following:

1. The ultimate analysis of the coal (C, H, O, N, S) expressed in wt%.

2. The proximate analysis of the coal (fixed carbon, volatile matter) expressed in wt%.

3. The heat of combustion of the fuel expressed in

Btu/lb - This value can be replaced by the high heating value (HHV) which is often reported in laboratory reports.

4. The excess air for combustion which is expressed in percent of theoretical air - For a pulverized-coal-fired system, excess air is usually between 15-30 percent.

5. Absolute humidity of air or water content per lb of dry air expressed in (lbs H_2O per lb air) - This value is normally determined from the psychrometric charts.

6. The inlet air temperature expressed in ^{O}C.

7. The inlet coal temperature expressed in ^{O}C.

8. The unburned combustible matter - There are two possible sources of such unburned material. The first and most important is the one due to the carbon which is trapped in the ash, usually expressed in wt% of ash (5-15%). The second source of unburned combustible is the incomplete combustion of the carbon in the fuel expressed in % carbon converted into CO.

Boiler Ash

The main difference between the ashing condition in the laboratory muffle furnace and that in the boiler plant is the coal combustion condition. The boiler ash usually reacts rapidly, therefore some unburned carbon remains trapped in the boiler ash. For low-volatile anthracite coals, the unburned carbon content may reach 15 percent (Raask 1985, g). Thus, the boiler ash is the laboratory-measured ash (ASTM ash) plus unburned carbon within the ash.

In this computer program this is denoted as

ASH = ASHLAB + ASHC.

Enthalpy Changes of the Inlet Coal Fuel

The enthalpy changes of the inlet coal are taken as the summation of the enthalpy changes of the individual components: carbon, volatile matter, inlet ash and moisture of the coal.

$$HCOAL = HFC + HVM + HASHI + HH_2OC.$$

These enthalpies can be calculated as

$$H_{T1} - H_{298} = n_i \int_{298}^{T1} C_{Pi}dT.$$

where n_i = moles of the i-th component in the feed or product.

C_{Pi} = heat capacity of the i-th component in the feed or product.

The instantaneous heat capacities as functions of temperature are listed as follows: (DOE, 1978)

Fixed carbon:

$$C_{PC} = 0.145+4.7*10^{-4}T-(2.63*10^{-7})T^2+(5.25*10^{-11})T^3.$$

Ash: $C_{ASH} = 0.182 + (7.78*10^{-5})T.$

Volatile matter:

$$C_{VM} = 0.4128 + 4.389*10^{-4}T.$$

where heat capacities are in cal/g^{0}K and T is in ^{0}K.

Enthalpy Changes of Inlet Air

The enthalpy changes of the inlet air are taken as the summation of the enthalpy changes of inlet oxygen, inlet nitrogen and the humidity of the inlet air. The gas heat capacities are shown as follows:(Reid, et al.,1977)

Oxygen:

$$C_{PO2} = 6.713-0.879*10^{-6}T+4.17*10^{-6}T^2-2.544*10^{-9}T^3.$$

Nitrogen:

$$C_{PN2} = 7.44-0.324*10^{-2}T+6.4*10^{-6}T^2-2.79*10^{-9}T^3.$$

$H_2O_{(g)}$:

$$C_{PH2O} = 7.701+4.595*10^{-4}T+2.521*10^{-6}T^2-0.859*10^{-9}T^3.$$

where heat capacities are in cal/g^{O}K and T is in ^{O}K.

The moles of inlet oxygen are the oxygen required during the combustion plus the amount of excess oxygen. This is expressed as:

```
O2R = O2TH*(1+P/100.0)
```

where P is the percentage of the excess air and

O2TH is the theoretical oxygen demand.

From the material balance on the combustion, the theoretical oxygen is calculated from the summation of the oxygen needed for the following reactions:

$$C + O_2 \text{ -----} \rightarrow CO_2$$

$2H + 1/2\ O_2 \longrightarrow H_2O$

$S + O_2 \longrightarrow SO_2$

The moles of inlet nitrogen are the moles of inlet oxygen times nitrogen to air ratio(79/21). This is expressed as:

NR = O2R(79/21)

The moles of water are calculated from the mole fraction of as water in the humid air (W) and is expressed as:

H2OO = (W * DAIR)/(1.0-W)

where DAIR = O2R+NR.

Thus, the enthalpy changes of the inlet air (HAIR) are calculated.

The Heat of Combustion and Energy Release of the Coal

The heat of combustion is the amount of heat generated by the complete combustion of a unit weight of coal. As long as the fuel is the same and the combustion is complete, the heat of combustion is a constant. This value is usually determined by direct measurement in a calorimeter of the heat evolved during combustion. This value may also be estimated by Dulong's formula.

$Btu/lb = 14544C+62028(H_2-O_2/8)+4050S$

In coal laboratory reports, the heating value is

usually reported. The heating value of a coal is the negative of the standard heat of combustion (25 ^{0}C). The higher heating value (HHV) is used to describe the heating value, when the water in the combustion product is considered as liquid and the lower heating value (LHV) is when water is a vapor in the product. In the United States usually the higher heating value is used in combustion calculations, while in Europe the lower heating value is normally used. In this case, since only water vapor is involved, the higher heating value from the laboratory report should be converted to the lower heating value.

$$LHV = HHV - 9W_H h_{fg} \quad (Btu/lb)$$

where LHV is the lower heating value of the fuel,

HHV is the higher heating value of the fuel,

h_{fg} is the heat of vaporization of water at 25^{0}C,

W_H is the hydrogen content of coal.

The actual energy released in the furnace above standard state and available for absorption in the furnace is equal to the lower heating value of the fuel minus the energy equivalent of the unburned fuel. This is calculated by:

$$ER = LHVT - HHV*0.0022*252*ASHC, \quad (cal)$$

where ER is total energy released from coal, cal,

LHVT is the total lower heating value, cal,

HHV is the higher heating value, Btu/lb,

ASHC is the unburned carbon content, g,

0.0022 is the conversion factor to convert lb into g,

252 is the conversion factor for Btu into cal.

Enthalpy Changes of the Products

The products of the combustion consist of the flue gases and the ash products. The flue gases are H_2O, CO_2, CO, SO_2, N_2 and O_2. From each stoichiometric equation, the moles of the flue gases can be determined. Again, by utilizing the specific heat capacity of each component, the enthalpy changes of the flue gases and the ash can be determined as a function of the flame temperature. The heat capacities of flue gases are listed as follows: (Reid et al.,1977)

Oxygen:

$$C_{PO2} = 6.713-0.879*10^{-6}T+4.17*10^{-6}T^2-2.544*10^{-9}T^3.$$

Nitrogen:

$$C_{PN2} = 7.44-0.324*10^{-2}T+6.4*10^{-6}T^2-2.79*10^{-9}T^3.$$

$H_2O_{(g)}$:

$$C_{PH2O} = 7.701+4.595*10^{-4}T+2.521*10^{-6}T^2-0.859*10^{-9}T^3.$$

CO:

$$C_{PCO} = 7.373-0.307*10^{-2}T+6.662*10^{-6}T^{-2}-3.037*10^{-9}*T^3$$

CO_2:

$C_{PCO2} = 4.728-1.754*10^{-2}T-1.338*10^{-5}T^2+4.097*10^{-9}T^3$

SO_2:

$C_{PSO2} = 5.697-1.6*10^{-2}T-1.185*10^{-5}T^2+3.172*10^{-9}T^3$

where heat capacities are in cal/g^{0}K and T is in K.

Energy Balance Within for Adiabatic Combustion

If the control volume is taken as the fired ball and steady state is assumed within the combustor, then the energy balance within this adiabatic reactor can be performed.

Rate of thermal energy in - rate of thermal energy out + rates of thermal energy produced = 0

$$\Delta H_{in} - \Delta H_{out} + Q_{combustion} = 0$$

where ΔH_{in} = enthalpy changes of the fuel and air input,

ΔH_{out} = enthalpy changes of the products,

$Q_{combustion}$ = energy released from the fuel.

Since the heat capacity equations of the gaseous components are higher than second order, the energy balance equation which is a function of the adiabatic flame temperature(T_{ad}) becomes a fourth order equation. This equation is solved by Newton-Raphson method. The algorithm is as follow:

1. Set an initial value for T_{ad}.

2. Insert Tad into energy balance equation and obtain a value (HAD).

3. Differentiate the energy balance equation and substitute with Tad and obtain a value for this differentiated equation (HADD).

4. Set $T_{new} = T_{ad} - HAD/HADD$.

5. If |Tnew - Tad| < tolerance, then procedure is completed successfully, otherwise set $T_{ad} = T_{new}$ and proceed to step 2.

Qualitative and Quantitative Determination of Deposits

From the mineral matter analyses, there are 10 elements (Fe, Ca, Mg, Na, K, Si, Al, Ti, S, P) which should be considered. For some European coals, Cl is also needed to be taken into consideration. During combustion, a range of mineral compounds are formed which may create deposits. These elements usually appear as oxides. However a suitable criterion must be selected to determine the extent of formation of each compound. Wibberley and Wall (1982) reported that the alkali deposits formed on the fly ash in large pulverized-coal-fired boilers are determined by thermodynamics rather than kinetic constraints. Other thermodynamic calculations have been used by Halstead and Raask (1969) and Smith et al. (1985) to predict the behavior of ash species during both pulverized-coal combustion and deposit formation. Still, application of their results to the highly complex systems present in many boilers remains uncertain.

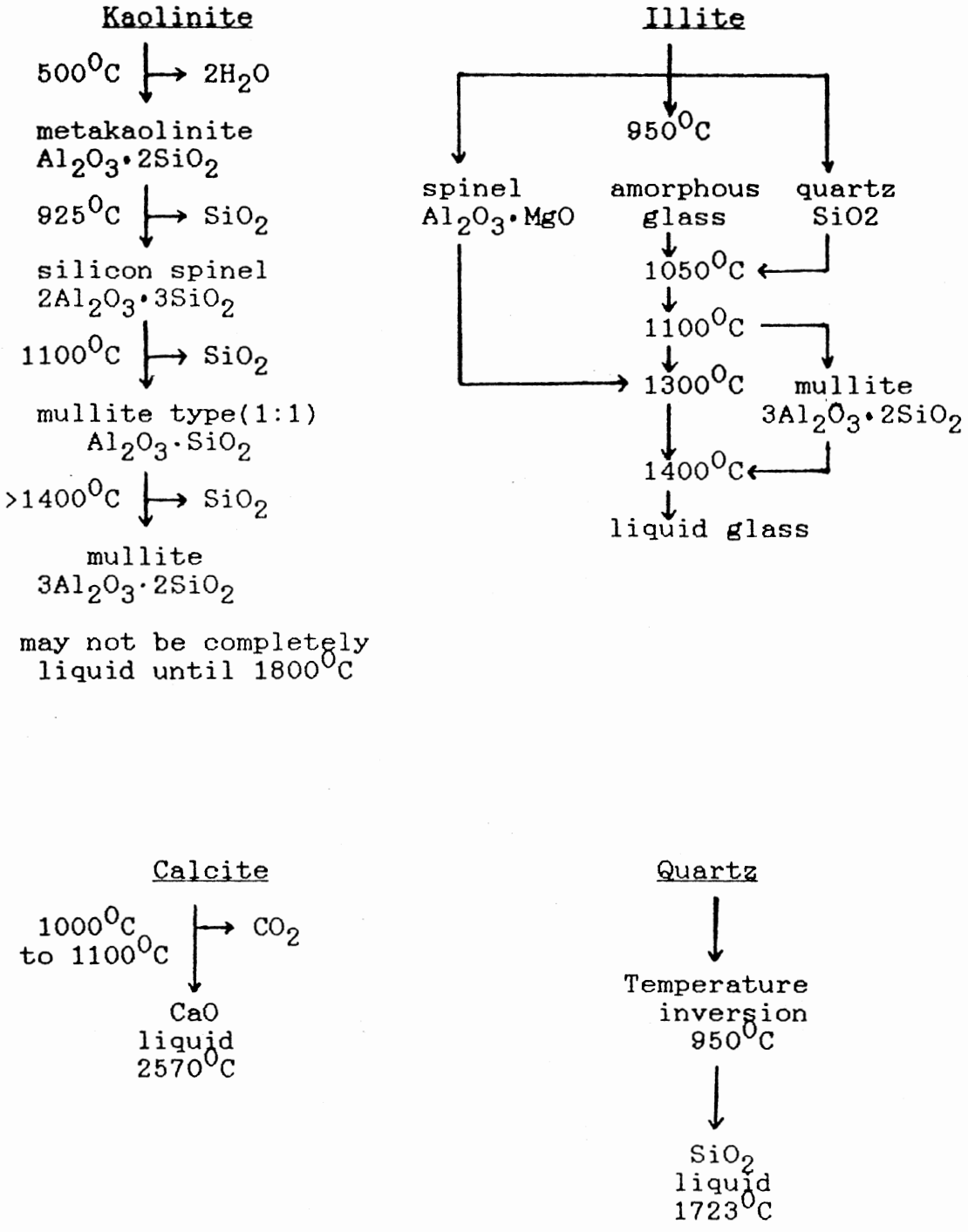
Determination of the major species of deposits formed from different elements present in the coal is considered here. Figure 6 summarizes the phase transformations which pure mineral matter commonly found in coals undergoes during heating (Bryer,1984). Also, Lewis(1978) reported the major crystalline mineral phases found in the pulverized coal combustion products are mullite ($Al_6Si_2O_{13}$), lime (CaO), magnetite (Fe_3O_4), hematite (Fe_2O_3), quartz (SiO_2) and anhydrite ($CaSO_4$).

Wibberley and Wall(1982) showed that alkalis and/or sulfur are most commonly associated with severe fouling. The relative order of stability of sodium compounds for the range of 1027 - 1727 ^{0}C is as follows:

$$NaCl > Na_2Si_2O_5 > NaOH.$$

Through thermodynamic calculations they suggest that sodium sulfate is also stable and at equilibrium will account for the total sodium content of the coal, providing sufficient sulfur is present. Anhydrite ($CaSO_4$) is also expected to be formed in the boiler, especially in the temperature range of 850 - 1000 ^{0}C (Drummond et al., 1977).

Thus, based on these studies, the major compounds possible in deposits are mullite ($Al_6Si_2O_{13}$), quartz (SiO_2), aluminum oxide (Al_2O_3), anhydrite ($CaSO_4$), sodium sulfate (Na_2SO_4) and hematite (Fe_2O_3). The amounts of these species can be quantified through the evaluation of their equilibrium constants.



(Bryer, 1984)

Figure 6. Phase Transformatin of Mineral Matters Commonly Found in Coal

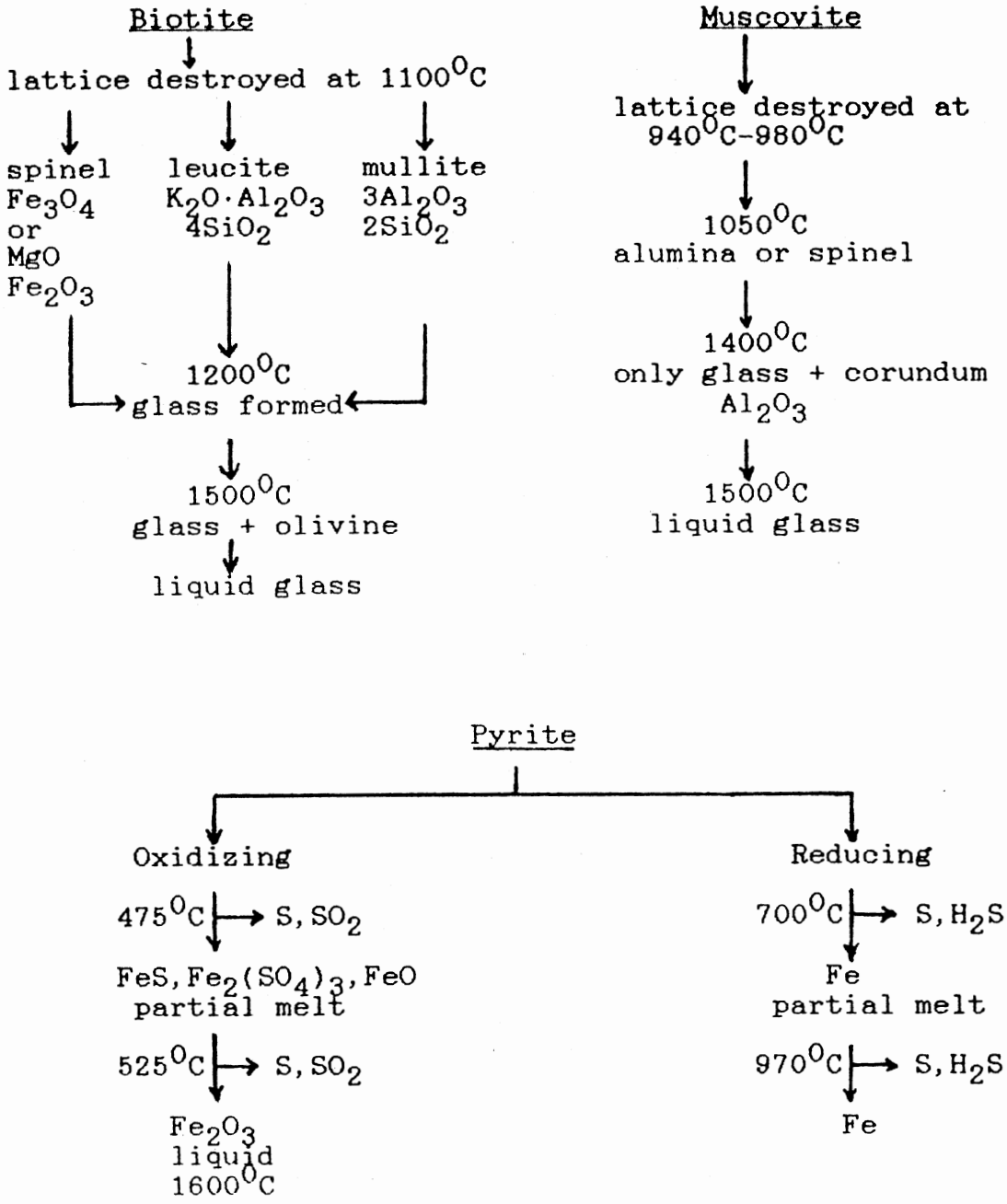


Figure 6. (Continued)

Evaluation of the Equilibrium Constants

The Gibbs energy of any substance is the maximum portion of its energy which can be converted into mechanical work under a given condition. If a reaction takes place a change in the Gibbs energy of the system will also occur. This change is equal to the net reversible work done by or absorbed during the reaction. The Gibbs energy can be given by the relationship

$$\triangle G = -RT\ln K_P + RT\ n\ln P$$

where n = the number of moles in the reaction,

P = reaction pressure,

K_P= equilibrium constant of the reaction,

If the pressure is 1 atm, then the term RT nlnP = 0, therefore,

$$\triangle G^0 = -RT\ln K_P.$$

where $\triangle G^0$ = standard Gibbs energy change of a reaction.

If mineral species are assumed to reach equilibrium, then the variation of equilibrium constants with temperature can determine the more stable mineral species. With an increase in equilibrium constant, the standard Gibbs energy change of the reaction becomes more negative, thus the reaction is more likely to occur and the product of this reaction will be more stable. Thus, for an element, considering the usually occurring chemical reactions at a

given temperature, the reaction with higher K_P value will have a more stable product than the one with lower K_P value. In determining the major species present under different conditions, the reactions have been chosen as comprehensively as possible by including as many species as possible and by carrying out the calculations over a wide range of temperatures and stoichiometries.

For Al and Si elements, the possible combinations of coal deposits are Al_2O_3, Al_2SiO_5, $3Al_2O_3$ $2SiO_2$ and SiO_2. Table VII (Stull and Prophet, 1971) shows the relations between the temperature and the equilibrium constant (K_P) of these compounds in the following reactions:

$$2Al + 3O_2 \longrightarrow Al_2O_3$$

$$Al_2O_3 + SiO_2 \longrightarrow Al_2SiO_5$$

$$3Al_2O_3 + 2SiO_2 \longrightarrow Al_6Si_2O_{13}$$

$$Si + O_2 \longrightarrow SiO_2$$

From this table, it is observed that the $Al_6Si_2O_{13}$ formation reaction possesses a higher equilibrium constant than the other reactions, thus it can be formed easily in the deposits. Furthermore, the equilibrium constant of $Al_6Si_2O_{13}$ is much larger than that of Al_2SiO_5, to simplify the case, one may assume that Al_2SiO_5 does not appear in deposits and mullite ($Al_6Si_2O_{13}$) is the only aluminosilicate formed, as long as there is excess of both Si and Al. Once,

TABLE VII

EQUILIBRIUM CONSTANTS AND TEMPERATURES FOR SOME COMMON REACTIONS OF Al, Si COMPOUNDS

M.P. (^{O}C)	Al_2O_3 2042	$Al_6Si_2O_{13}$ 1750	Al_2SiO_5 1545	SiO_2 1423
Temp(^{O}K)	log(K_p)	log(K_p)	log(K_p)	log(K_p)
298	277.13	1128.60	428.18	150.00
500	158.61	646.17	244.64	85.62
600	129.44	527.43	199.47	69.77
700	108.62	442.65	167.23	58.46
800	93.01	379.11	143.06	49.99
900	80.88	329.72	124.27	43.41
1000	71.09	289.98	109.17	38.15
1100	63.06	257.40	96.79	33.85
1200	56.40	230.23	86.48	30.28
1300	50.70	207.28	77.77	27.25
1400	45.90	187.62	70.30	24.66
1500	41.70	170.59	63.84	22.42
1600	38.00	155.70	58.20	20.46
1700	34.80	142.55	53.21	18.72
1800	32.00	130.73	48.70	17.10
1900	29.4	120.15	44.68	15.65
2000	27.0	110.65	41.06	14.35
2100	25.0	102.06	37.79	
2200	23.0	94.26	34.83	
2300	21.4	87.14	32.12	
2400	19.8	80.62	29.65	
2500	18.3	74.63	27.38	
2600	17.0	69.11	25.28	
2700	15.8	64.00	23.35	
2800	14.4	58.88	21.42	
2900	12.9	53.35	19.39	
3000	11.6	48.20	17.49	

(Stull and Prophet, 1971)

one of these elements is completely consumed the excess of the other element, Si or Al may be assigned to SiO_2 or Al_2O_3, as the case may be.

Despite the fact that sodium is a minor constituent in the ash, it has been generally found that the alkali layer of ash deposit is rich in the volatile elements: sodium and sulfur. Table VIII (Stull and Prophet, 1971) lists various equilibrium constants at different temperatures for the following equations:

$$Na_2CO_3 + SiO_2 \longrightarrow Na_2SiO_3 + CO_2$$

$$2Na + Hg_2SO_4 \longrightarrow 2Hg + Na_2SO_4$$

$$2NaOH \longrightarrow Na_2O + H_2O$$

$$Na_2O + CO_2 \longrightarrow Na_2CO_3$$

Since Si has already been assigned as mullite and quartz, there is no excess Si to form Na_2SiO_3. As for Na_2CO_3 and Na_2SO_4, Na_2SO_4 is more stable than Na_2CO_3. Thus Na_2SO_4 is chosen as the possible deposit. For coal with significant amounts of Cl, NaCl is the first compound to be considered (Drummomd et al., 1977). From the above discussion, it is concluded that NaCl and Na_2SO_4 are the stable compounds present in the ash deposits.

In dealing with Ca, equilibrium constants can not be found in literatute, however, standard Gibbs energy can be applied.

TABLE VIII

EQUILIBRIUM CONSTANTS AND TEMPERATURES FOR SOME COMMON REACTIONS OF Na COMPOUNDS

M.P. (^{O}C)	Na_2O 1132	Na_2CO_3 850	Na_2SiO_3 1089	Na_2SO_4 884
Temp(^{O}K)	log(K_P)	log(K_P)	log(K_P)	log(K_P)
298	66.42	183.62	257.00	221.75
500	36.65	103.48	257.08	123.92
600	29.29	83.75	119.15	99.80
700	24.04	69.70	99.69	82.59
800	20.12	59.21	85.11	70.05
900	17.08	51.08	73.79	59.66
1000	14.66	44.59	64.76	51.38
1100	12.69	39.30	57.38	38.87
1200	10.90	34.75	51.07	44.63
1300	8.90	30.42	45.25	33.50
1400	7.22	26.73	40.27	28.93
1500	5.76	23.55	35.97	24.99
1600		20.80	32.22	21.57
1700		18.38	28.91	18.57
1800		16.25	25.91	15.91
1900		14.36	23.24	13.55
2000		12.67	20.84	11.44
2100			18.68	
2200			16.73	
2300			14.95	
2400			13.33	
2500			11.85	

(Stull and Prophet, 1971)

$CaSO_4$: $Ca + S + 2O_2 \longrightarrow CaSO_4$

$\Delta G^0 = -33640+15.91T\log T-5.94*10^{-3}T^2-1.093*10^5T^{-1}+46.02$

(Kelley, 1937)

$CaCO_3$: $CaO + CO_2 \longrightarrow CaCO_3$

$\Delta G^0 = -40250+34.4T$ (Kubaschewski and Alcock, 1981).

CaO: $Ca + 1/2\ O_2 \longrightarrow CaO$

$\Delta G^0 = -151325+23.66T$ (Kubaschewski and Alcock, 1981).

$Ca_3(PO_4)_2$: $3CaO + P_2O_5 \longrightarrow Ca_3(PO_4)_2$

ΔG^0 can be read directly from Kelley(1943). From these standard Gibbs energies, equilibrium constants are calculated at different temperatures and are tabulated in Table IX. The relative stability of calcium compounds can be summarized in the following order: $Ca_3(PO_4)_2$ > $CaSO_4$ > CaO > $CaCO_3$. Therefore, Ca was assigned to $Ca_3(PO_4)_2$, $CaSO_4$ and CaO in this project.

Thus by considering the stable compounds of sodium and calcium all the possible sulfate and phosphate compounds are determined, therefore the other elements can be considered mainly as oxides. Table X (Stull and Prophet, 1971) shows the equilibrium constants of Fe, Mg and Ti compounds at different temperatures under the following reactions:

$3Fe + 4H_2O \longrightarrow Fe_3O_4 + 4H_2$

$4Fe_2O_3 + O_2 \longrightarrow 6Fe_2O_3$

$Mg + 1/2\ O_2 \longrightarrow MgO$

TABLE IX

EQUILIBRIUM CONSTANTS AND TEMPERATURES FOR SOME COMMON REACTIONS OF Ca COMPOUNDS

M.P. (^{O}C)	$CaSO_4$ 1450	CaO 2614	$Ca_3(PO_4)_2$ 1670	$CaCO_3$ 1339
Temp(^{O}K)	log(K_p)	log(K_p)	log(K_p)	log(K_p)
298	228.9	105.9	737.0	22.0
500	128.6	61.0	445.7	10.1
600	103.8	50.0	374.5	7.2
700	86.0	42.1	324.6	5.1
800	72.9	36.2	287.2	3.5
900	62.6	31.6	258.4	2.7
1000	54.4	27.9	235.5	1.3
1100	47.7	24.9		0.5
1200	42.1	22.4		- 0.2
1300	35.7	20.3		- 0.8
1400	33.4	18.5		
1500	29.9	16.9		
1600	26.8	15.5		
1700	24.2	14.3		
1800	21.8	13.2		
1900	19.7	12.2		
2000	17.9	11.4		
2100	16.2			
2200	14.6			
2300	13.2			
2400	11.9			
2500	10.8			
2600	9.7			
2700	8.8			
2800	7.9			
2900	7.0			
3000	6.3			

TABLE X

EQUILIBRIUM CONSTANTS AND TEMPERATURES FOR SOME COMMON REACTIONS OF Fe, Ti AND Mg COMPOUNDS

M.P. (^{o}C)	Fe_2O_3 1462	Fe_3O_4 1597	TiO_2 1870	Ti_2O_3 1839	MgO 2825
Temp(^{o}K)	log(K_p)	log(K_p)	log(K_p)	log(K_p)	log(K_p)
298	130.3	178.3	155.8	251.3	99.7
500	93.5	99.1	89.0	143.8	57.2
600	72.0	79.7	72.6	117.5	46.7
700	57.7	66.0	60.9	98.7	39.2
800	47.5	55.7	52.1	84.6	33.6
900	40.0	47.8	45.3	73.7	29.3
1000	34.1	41.4	39.8	65.0	25.7
1100	29.4	36.2	35.3	57.8	22.9
1200	25.5	31.9	31.6	51.9	20.4
1300	22.3	28.2	28.4	46.9	18.4
1400	19.6	25.1	25.7	42.6	16.6
1500	17.3	22.4	23.4	38.9	14.8
1600	13.5	20.0	21.4	35.6	13.2
1700	12.0	17.9	19.6	32.8	11.7
1800	10.6	16.0	18.0	30.2	10.5
1900	9.3	14.3	16.5	28.0	9.4
2000	8.2	12.7	15.2	26.0	8.4
2100	7.2	11.3	14.0	24.0	7.5
2200	6.2	10.0	13.0	22.3	6.7
2300	5.4	8.9	12.0	20.8	5.9
2400	4.6	7.8	11.1	19.3	5.2
2500	3.8	6.8	10.3	18.0	4.6
2600		5.9		16.8	4.0
2700		5.0		15.7	3.5
2800		4.2		14.7	3.0
2900		3.5		13.7	2.5
3000		2.8		12.8	2.1

(Stull and Prophet, 1971)

$Ti + O_2 \longrightarrow TiO_2$

$2TiO_2 \longrightarrow Ti_2O_3 + 1/2\ O_2$

Under identical conditions, the equilibrium constant of Fe_3O_4 is higher than that of Fe_2O_3. However, Rassk (1986,h) shows that in an oxidizing atmosphere, iorn oxide can exist both as mangetite (Fe_3O_4) and hematite (Fe_3O_4). Therefore, in this project, the iorn is assumed to be divided into equal moles of Fe_2O_3 and Fe_3O_4. Similarly, the equilibrium constants show that Ti_2O_3 is more stable than TiO_2, but in most literature sources it is reported that Ti exists as rutile (TiO_2). Therefore in this project, the element Ti is equally assigned as TiO_2 and Ti_2O_3.

The equilibrium constants of formation of potassium compounds are shown in Table XI (Stull and Prophet, 1971). From this table, K_2CO_3 can be selected as the stable compound during the formation of ash deposits.

In summary, both from previous literature surveys and from equilibrium constants studies, the major ash deposits are specified as $Al_6Si_2O_{13}$, Al_2O_3, SiO_2, NaCl, Na_2SO_4, $Ca_3(PO_4)_2$, $CaSO_4$, CaO, Fe_2O_3, Fe_3O_4, TiO_2, Ti_2O_3, MgO, and K_2CO_3.

Temperature Profile of a Boiler

In order to determine the formation environment of the ash deposits in a pulverized-coal-boiler, a suitable temperature profile of the boiler is needed. In the past,

TABLE XI

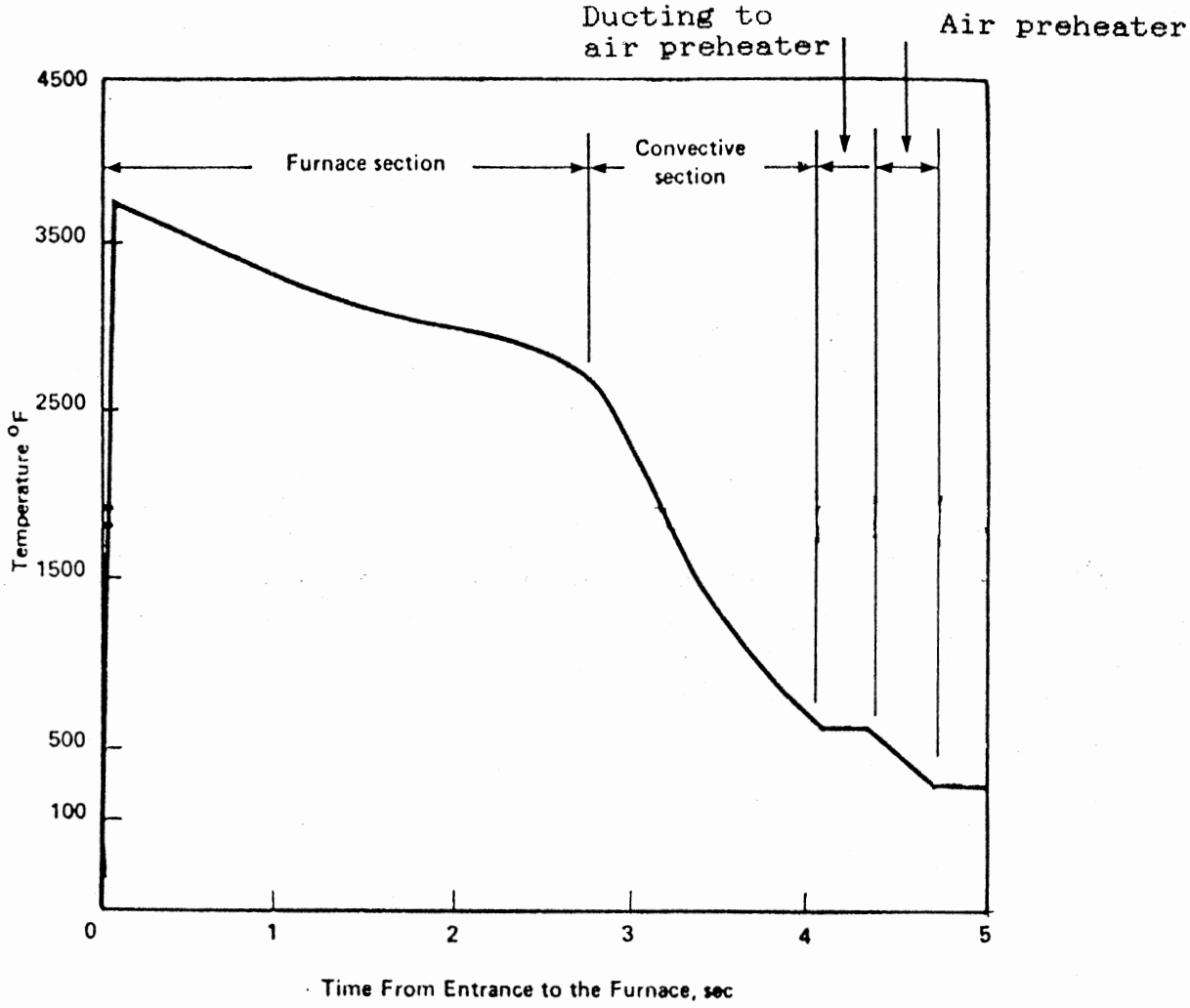
EQUILIBRIUM CONSTANTS AND TEMPERATURES FOR SOME COMMON REACTIONS OF K COMPOUNDS

	KCl	K_2CO_3	K_2O
M.P. (^oC)	771	901	881
T (^oK)	log(K_p)	log(K_p)	log(K_p)
298	71.6	186.5	56.4
500	40.6	105.0	30.6
600	33.0	84.9	24.2
700	27.6	70.6	19.7
800	23.5	59.9	16.4
900	20.4	51.6	13.8
1000	17.8	45.0	11.7
1100	15.6	39.2	9.7
1200	13.6	34.1	7.7
1300	11.9	29.9	6.0
1400	10.5	26.3	4.6
1500	9.2	23.1	3.4
1600		20.4	2.4
1700		18.1	1.5
1800		16.0	0.7
1900		14.2	0.3
2000		12.5	0.0

(Stull and Prophet, 1971)

comprehensive modeling of a pulverized-coal-boiler has been restricted by the lack of computer speed and by technical difficulties in describing essential model elements. Recently, modeling of complex coal furnaces has become of great interest to many investigators. A classification of models developed for coal flames in a boiler is summarized in Table XII (Smoot and Smith, 1985). Complete modeling of pulverized-coal combustor must account for all of these aspects. However, for this specific application, to consider all of these aspects will be complex and tedious, therefore, a simple and approximate method is developed to account for the temperature distributuin in the boiler. In this work, a typical temperature profile in a utility boiler is utilized to serve as a default temperature profile which is shown in Figure 7 (Howard, 1965). In this figure, the radiative section and the convective section are the main concern. If the combustion gas velocity in the boiler chamber is chosen to be 60 ft/sec (Singer, 1981), then the relations between temperature and residence time can be converted into the relations between temperature and the height of a boiler.

In order to properly apply this temperature profile in the computer model, it is necessary to convert this figure into equations. Simple linear regression is chosen to fit this figure and two equations are obtained to represent the temperature distributions of the radiative and convective sections.



(Howard, 1965)

Figure 7. Typical Temperature Profile Through a Utility Boiler

TABLE XII

CLASSIFICATION OF PRACTICAL COAL FLAMES

Flow Type	Process Application	Typical Flame Type	Typical Mathematical Complexity
Perfectly stirred reactor	Fluidized bed	Well mixed, kinetically controlled	Zero dimensional
Plug flow	Moving beds Steady fixed beds	Solid reaction/ heat transfer control	One-dimensional steady
Plug flow	Pulverized-coal furnace Entrained gasifier	Mixing specified	One-dimensional steady
Plug flow	Coal mine explosions Coal process explosions Flame ignition	Premixed flame Kinetic and diffusion control	One-dimensional transient
Recirculating flow	Power generators Entrained gasifiers Industrial furnaces	Diffusion flames, complex control	Multi-dimensional steady or transient

(Smoot and Smith, 1985)

Since the calculated flame temperature of coal is different from the peak temperature shown in this figure, a ratio between these two temperatures is introduced to normalize the temperature distribution equations.

Another option to determine the temperature profile is to use the in temperatures at different locations in the boiler which can be measured by a pyrometer, as input data to the computer program. Following regression method, the temperature profile equations can be found.

Vapor Pressure of Mineral Species

When the determined mineral species are heated at flame temperature, they tend to partially vaporize. The system pressure can be calculated from Dalton's Law:

$$P_{Total} = P_{Flue\ gas} + P_{Mineral\ Vapor}.$$

Since partial pressure of the mineral species is determined by their vapor pressure, the vapor pressure equations are needed to calculate these partial pressures. After that, the mineral species in the vapor phase can be determined by the ideal gas law.

Some high temperature vapor pressure data of inorganic substances can be found in Kelly(1935), Stull(1947) and Kubaschewski(1979). Some vapor pressure equations found in the literatures are listed here.

Al_2O_3: melting point 2042 ^0C (Samonov, 1982)

$\log P_{Pas} = 13.42-27320.0/T$ (range 2327 - 2627 ^0C)

Fe_3O_4: melting point 1597 ^{O}C (Samonov, 1982)

$\log P_{Pas} = 14.24-22780.0/T$

CaO: melting point 2572^{O}C (Samonov, 1982)

$\log P_{Pas} = 12.85-28020.0/T$ (range 727 - 2587 ^{O}C)

TiO_2: melting point 1870 ^{O}C (Samonov, 1982)

$\log P_{Pas} = 14.37-30060.0/T$

Ti_2O_3: melting point 1839 ^{O}C (Samonov, 1982)

$\log P_{Pas} = 31.68-64700.0/T-1.26*10^{-3}T$ (range 1698 - 1878^{O}C)

MgO: melting point 2825^{O}C (Samonov, 1982)

$\log P_{Pas} = 12.37-26100.0/T$

Na_2SO_4: melting point 884^{O}C (Lovering, 1983)

$\log P_{atm} = 5.37-1.27*10^{-4}/T$ (range 1069 -1395^{O}C)

NaCl: melting point 801^{O}C (Janz, 1967)

$\log P_{mmHg} = -11495/T-3.526\log T+20.929$

SiO_2: melting point 1423^{O}C (Weast et al., 1987)

$\log P_{mmHg} = 13.43-26428.38/T$

K_2CO_3: melting point 901^{O}C (Stern and Weise, 1969)

$\log P_{atm} = 5.39-12700.0/T$ (range 764 - 911 ^{O}C)

However, the vapor pressure data for $Al_6Si_2O_{13}$, $CaSO_4$, $Ca_3(PO_4)_2$ and Fe_2O_3 could not be found in the literature. Therefore an estimation technique has to be used to obtain the vapor pressures of these compounds.

Estimation of Vapor Pressure

The Clausius - Clapeyron equation is the fundamental equation to estimate the vapor pressure of a condensed phase which is expressed as:

$$d\ln P = \frac{\Delta H_v}{RT^2} dT$$

where P is saturated pressure of a condensed substance(atm),

ΔHv is the heat of vaporization of a condensed substance (J/gmole),

R is the gas constant, 8.314 J/gmole·K,

T is the temperature (K).

As equilibrium is maintained between the vapor phase and the condensed phase, P is the saturated vapor pressure exerted by the condensed phase at temperature T. H_v can be obtained by the specific heat of the gas minus the specific heat of the condensed phase(Gaskell,1981). If $\Delta C_p = \Delta a + \Delta bT - \Delta cT^{-2}$, then the heat of vaporation is $\Delta H_v = \Delta H_0 + \Delta aT + \Delta bT^2/2 + \Delta c/T$. By integrating the Clausius-Clapeyron equation, a vapor pressure and temperature relationship for a particular substance can then be obtained. The normal boiling point, which is the temperature at which the vapor pressure

becomes equal to 1 atm, can be used as a boundary condition to determine the integration constant.

This method of vapor pressure estimation requires vapor and solid or liquid specific heat equations and the boiling point of the compound. However for the ash deposit compounds of our interest these properties could not be found. When the difference in specific heat between gas and liquid or gas and solid is not available, it is customary to take the difference in specific heat between the two phases as zero (Kelly, 1935). This considers the heat of vaporization as a constant. In the case of the four compounds of interest in this project, not only the heats of vaporization but also the boiling points are not available. Therefore another approach must be used to estimate the vapor pressure equations.

According to Trouton's rule (Brewer, 1946), the entropy of vaporization is approximately constant.

$$\Delta S_v = (\Delta H_v)/T$$

where T = boiling point of the substance K,

ΔS_v = the entropy of vaporization,

ΔH_v = the enthalpy of vaporization.

Kelly(1935) surveyed liquid halides and showed that the entropy of vaporization is about 24 cal/mol^{O}K. Following this rule, if the boiling point of the desired compound can be obtained, and the entropy of vaporization of the compound can be estimated from those of similar group

compounds, the enthalpy of vaporization can be calculated. Then from Clausius-Clapeyron equation, the approximate vapor pressure equation can be obtained.

The boiling points and heats of vaporization of the metals of interest are listed as follows:

$Al(l)$ ----- $Al(g)$ boiling point = 2057 ^{0}C

$\triangle H_v$ = 61022 cal/gmol $\triangle S$ = 26 cal/gmol^{0}K

$Ca(l)$ ----- $Ca(g)$ boiling point = 1487 ^{0}C

$\triangle H_v$ = 36577 cal/gmol $\triangle S$ = 21 cal/gmol^{0}K

$Fe(l)$ ----- $Fe(g)$ boiling point = 2735 ^{0}C

$\triangle H_v$ = 84620 cal/gmol $\triangle S$ = 28 cal/gmol^{0}K

Using these S's and assuming that the boiling points of oxides and salts are 727^{0}C higher than the melting points, the vapor pressure equations can be developed. These predicted vapor pressure equations for the four compounds of interest are listed here.

$Al_6Si_2O_{13}$: T_m = 1750 ^{0}C, $\triangle H_v$ = 78598 cal/gmol

$$\ln P_{atm} = -39552.3468/T+13.08$$

$CaSO_4$: T_m = 1400 ^{0}C, $\triangle H_v$ = 56133 cal/gmol

$$\ln P_{atm} = -28247.4348/T+10.5677$$

$Ca_3(PO_4)_2$: T_m = 1730 ^{0}C, $\triangle H_v$ = 63063 cal/gmol

$$\ln P_{atm} = -31734.7734/T+10.5677$$

Fe_2O_3: T_m = 1462 ^oC, ΔH_v = 76580 cal/gmol

$$\ln P_{atm} = -38536.8397/T+14.0925$$

The validity of this estimation technique is check by calculating the vapor pressure of Fe_3O_4. The predicted vapor pressure is:

Fe_3O_4: T_m = 1597 ^oC, ΔH_v = 80360 cal/gmol

$$\ln P_{atm} = 14.0925-40438.9974/T$$

The vapor pressures calculated from this equation when compared with those calculated from the vapor pressure correlation indicate 39% and 76% error at 2000 K and 1500 K respectively.

Distribution of Deposits

Pulverized coal fired boilers usually operate at pressures slightly lower than atmospheric pressure. At high temperatures of combustion, the combustion system in the boiler may be assumed to follow ideal gas law. Therefore, using the equilibrium conversions and the estimated vapor pressures and assuming ideal gas the possible deposits at various heights can be calculated.

Hottel and Cohen(1958) developed a zonal method to analyze the heat flux and temperature distribution. In this method the combustion reactor was divided into a number of volumes and each volume was assumed to be perfectly mixed.

Therefore at steady state, each stage was assumed to have uniform properties and a single temperature. Based on this concept, if the furnace is divided into sections with equal volume, then at the same height each stage will have the same temperature and mineral matter distribution.

The simulation model in this project is developed considering that 100 grams of the pulverized coal are burned in a steady state combustor. The coal combustion is assumed to be instantaneous. Thus a combustion temperature is calculated for the given conditions of combustion. At this temperature, some of the mineral matters are vaporized or at least partially vaporized while the remainder falls to the bottom of the boiler as the bottom ash. As the flue gases rise, the temperature decreases. The vaporized minerals start to condense and attach to the water wall of the boiler. The volume of the flue gas can be determined by assuming 760 mm Hg of pressure in the combustion chamber and from the prevailing temperature profile. The partial pressures of mineral vapors are determined from the saturated vapor pressures of the specified compounds. Following the ideal gas law and starting from the highest temperature stage, the moles of mineral components in the vapor phase (N_v) can be calculated. For each inorganic compound, N_v is the maximum amount of the compound that can exist in the vapor phase.

$$N_v = P_v V/RT,$$

where

P_v: partial pressure of minerals in a specified zone(mm Hg),

V : volume of flue gas (lit),

R : gas constant, 62.36 mmHg l/gmol ^{O}K,

T : temperature in a specified zone(^{O}K).

The next step is to compare the moles available for a particular mineral compound with the moles in the vapor phase(N_v). If $N_a > N_v$, there should be N_v moles in the vapor phase and the difference of N_a and N_v is denoted as the moles of residual(N_n) that can condense in this stage. If $N_a < N_v$, all the mineral (N_a) will remain in the vapor phase and there will be no condensation of this compound in this stage. Therefore, in the first stage there will be N_n moles of residual matter formed while N_v moles of vapor may continue to move upward to the second stage.

In the second stage, from temperature profile and vapor pressure equations, vapor and solid distribution can be obtained following the same method as described for the first stage. By repeating this procedure for every stage, until the end of the convective zone, distribution of the deposits on the boiler walls can be obtained. After determining the amount of each mineral species in the vapor and solid phases, the composition of deposit at each stage is calculated and presented in form of ASTM ash analysis.

A parameter called slagging flux is also defined. This is the total rate of deposit build up per unit area of the wall in each stage. The surface area in a stage is

calculated from its width, length and height. The width and the length of a zone are specified from the dimensions of the boiler and the height of each zone is chosen as 10 feet.

The overall fuel consumption rate is needed to scale up the results from 100 grams of coal to the actual fuel throughput and to obtain the actual rate of accumulation of deposits. From this deposition rate and the surface area, the slagging flux in each zone can be determined. The computer code which is written in FORTRAN is listed in Appendix A and a sample of input-output data is shown in Appendix B. The numerical results of the model are transferred into a LOTUS 123 file and the final tabular results and plots are prepared. These results will be presented and discussed in the next chapter.

CHAPTER IV

RESULTS

In this study, two kinds of coals are considered. The analyses of two Wyoming coals, Jacobs Ranch and Clovis Point, are shown in Table XIII. From these coal analyses and the excess air as the input data, the following information can be obtained using the computer model described in the previous chapter.

1. The composition of the flue gas in the boiler
2. The wt % of boiler ash in the boiler
3. The adiabatic flame temperature in combustor
4. The distribution of vapor and ash deposition at various locations of the boiler
5. The slagging flux at different locations in the boiler
6. The composition of ash deposited at different locations in a boiler.

In the first case, the combustion of a Jacobs Ranch coal with air entering at 300 K and 0 to 50 percent excess air is considered. Figure 8 shows the relationship between the adiabatic combustion temperature and the amount of excess air. As expected, the coal combustion temperature decreases with increasing percent excess air. Figure 9

TABLE XIII

JACOBS RANCH AND CLOVIS POINT COAL ANALYSES

Coal Type (As Received)	Jacobs Ranch	Clovis Point
Proximate Analysis Wt.%		
Moisture	25.44	31.32
Volatile Matter	36.55	33.85
Ash	6.81	6.14
Fixed Carbon	31.20	28.69
Heating Value Btu/lb	8863.00	8014.00
Ultimate Analysis Wt.%		
Sulfur	0.64	0.43
Carbon	48.43	44.21
Hydrogen	3.96	3.52
Nitrogen	0.69	0.60
Oxygen	14.03	13.78
Chlorine	0.00	0.00
Moisture	25.44	31.32
Ash	6.81	6.14
Mineral Analysis Wt.%		
Iron as(Fe_2O_3)	7.15	4.29
Calcium as (CaO)	14.22	14.64
Magnesium as (MgO)	3.15	3.12
Sodium as (Na_2O)	0.68	1.08
Potassium as (K_2O)	1.37	1.45
Silicon as (SiO_2)	46.38	50.24
Aluminum as (Al_2O_3)	13.81	13.55
Titanium as (TiO_2)	1.15	0.95
Phosphorus as (P_2O_5)	1.11	1.56
Sulfur as (SO_3)	6.05	4.53

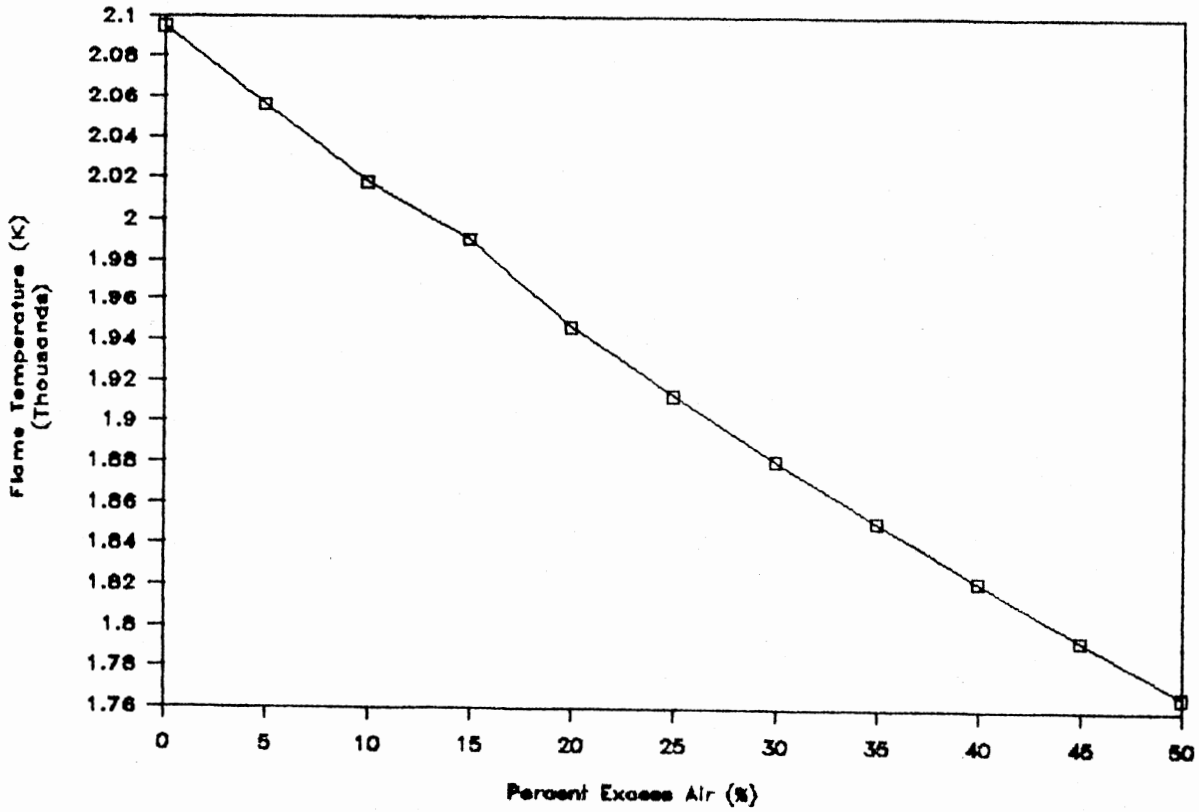


Figure 8. Flame Temperature at Various Percent Excess Air

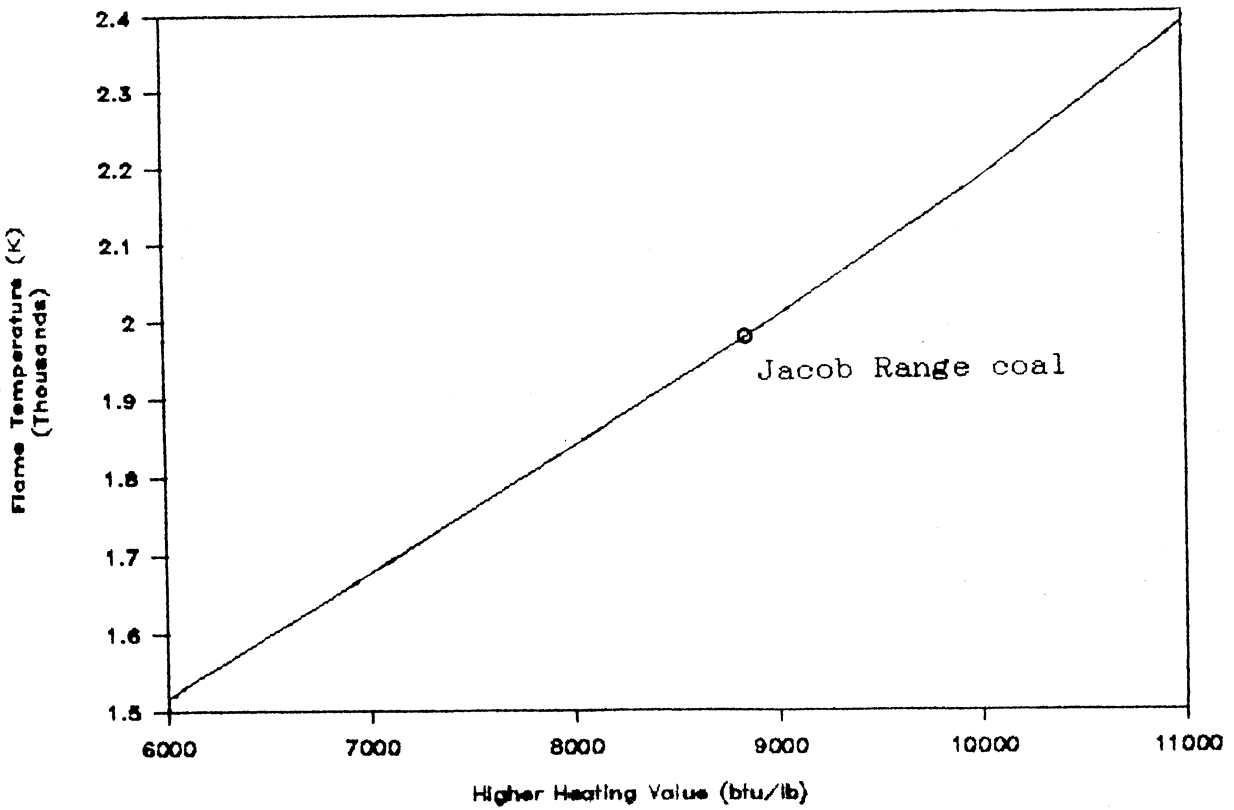


Figure 9. Flame Temperature at Various Heating Value

shows the effect of the heating value on combustion temperature for the Jacobs Ranch coal with 15% excess air at 300 K and varying higher heating values from 6000 to 12000 Btu/lb. Again, as expected, the adiabatic flame temperature increase with the heating value of the coal. Figures 10 to 22 show the distribution of each mineral in the vapor and ash deposits at different locations in the boiler. From these figures, the following results can be concluded:

1. The more refractory oxides such as Al_2O_3, TiO_2, Ti_2O_3, SiO_2, CaO, and MgO will tend to condense in the lower part of the boiler. After accumulation and spalling processes, these oxides become the major sources of the bottom ash.

2. In the middle parts of the boiler, mullite, Fe_2O_3 and Fe_3O_4 are the dominant compounds of ash deposition.

3. At low temperature zones, Na_2SO_4, K_2CO_3, $Ca_3(PO_4)_2$, and $CaSO_4$ are the major compounds of the ash deposits.

The ash deposit distributions for Jacobs Ranch (JR), Clovis Point (CR) and on a blend of 50% JR - 50% CP coals as input fuel are shown in Figures 23 to 27. Since the ash analyses of these two coals are very similar, this simple model does not show any great difference in the deposit compositions. The engineers of the Public Service Company of Oklahoma at the Oolagah power plant have observed that a 50-50 blend of the two coals causes more boiler deposition and fouling than either of the two pure coals. Therefore, other factors, besides regular coal analysis should be

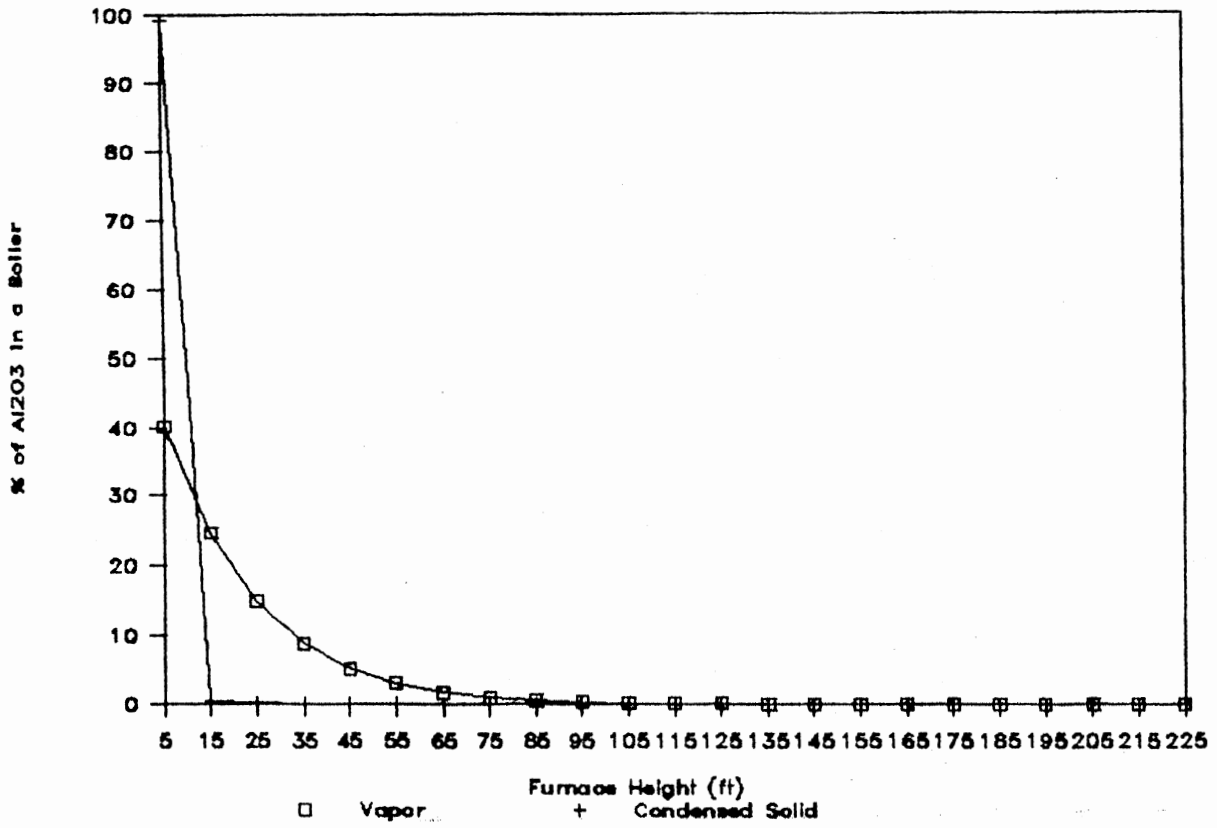


Figure 10. Distribution of Al_2O_3 at Different Locations

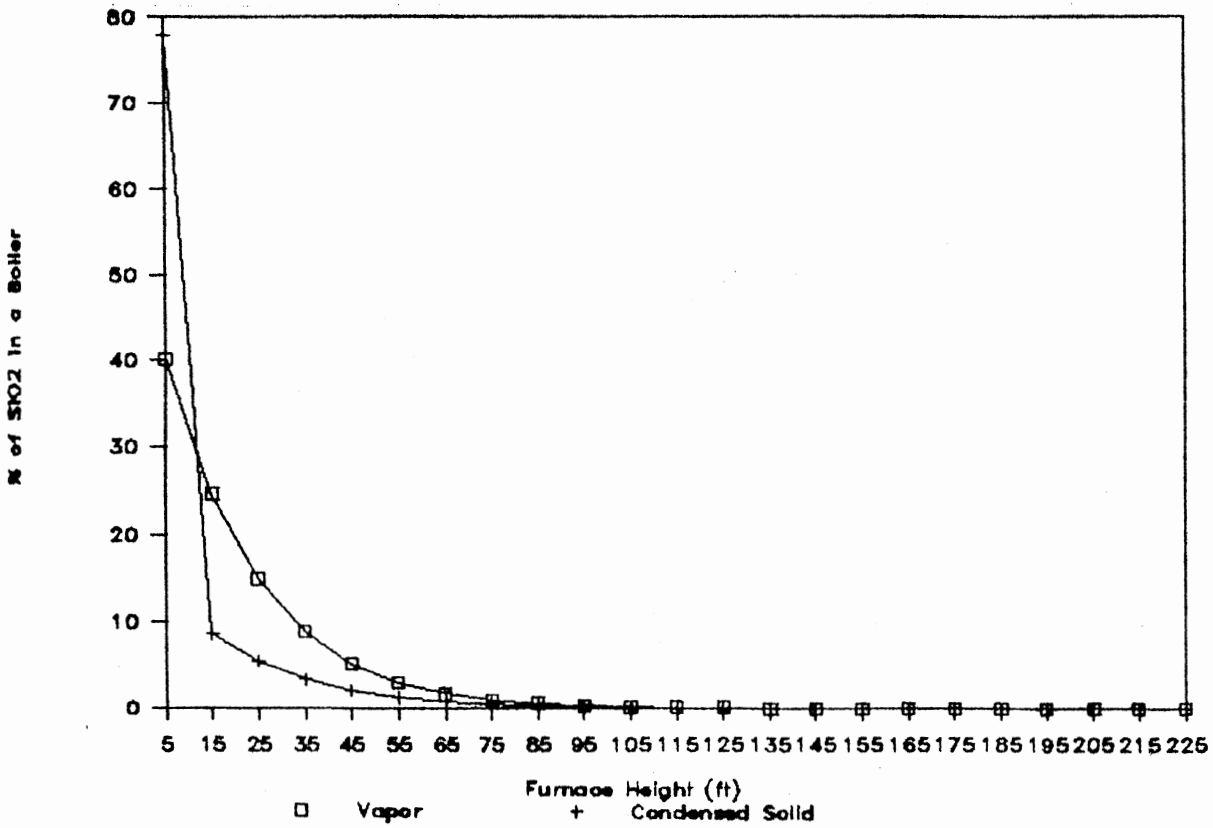


Figure 11. Distribution of SiO_2 at Different Locations

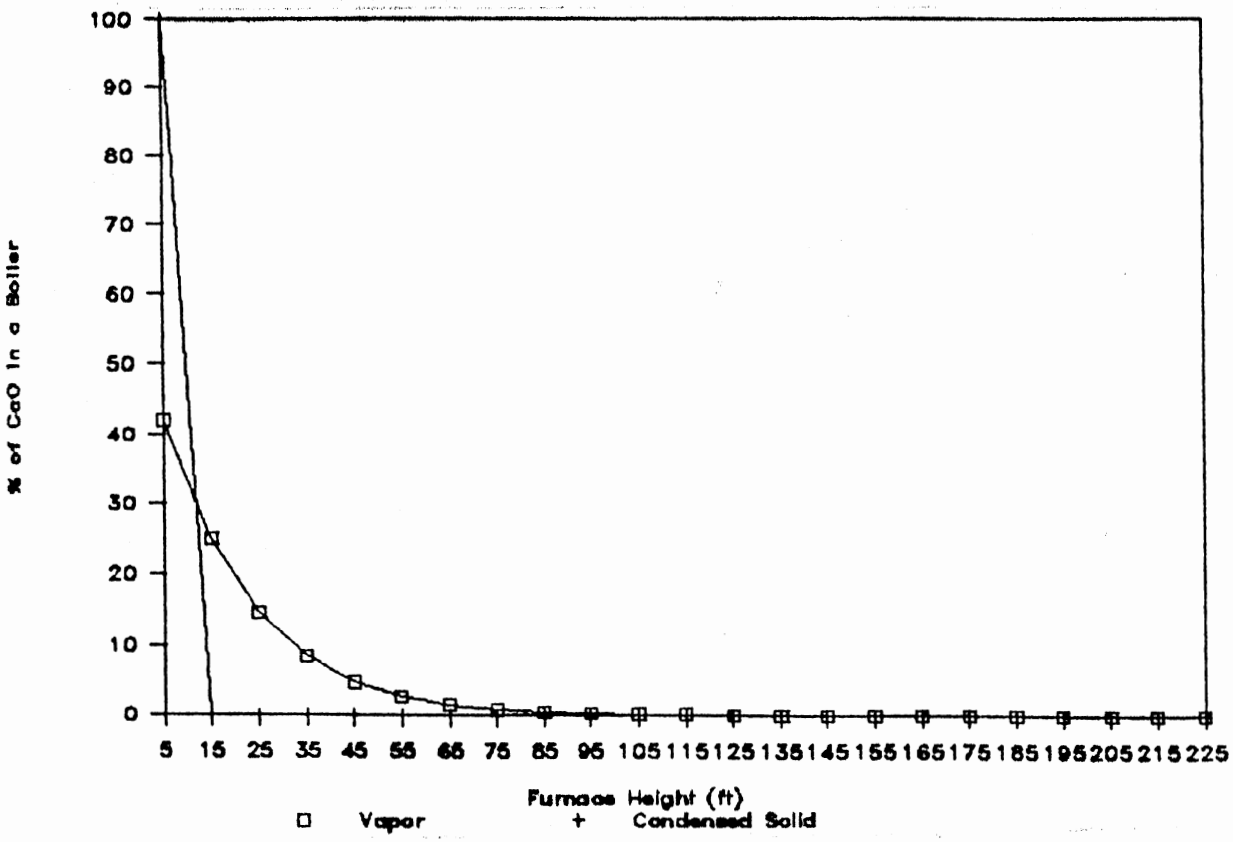


Figure 12. Distribution of CaO at Different Locations

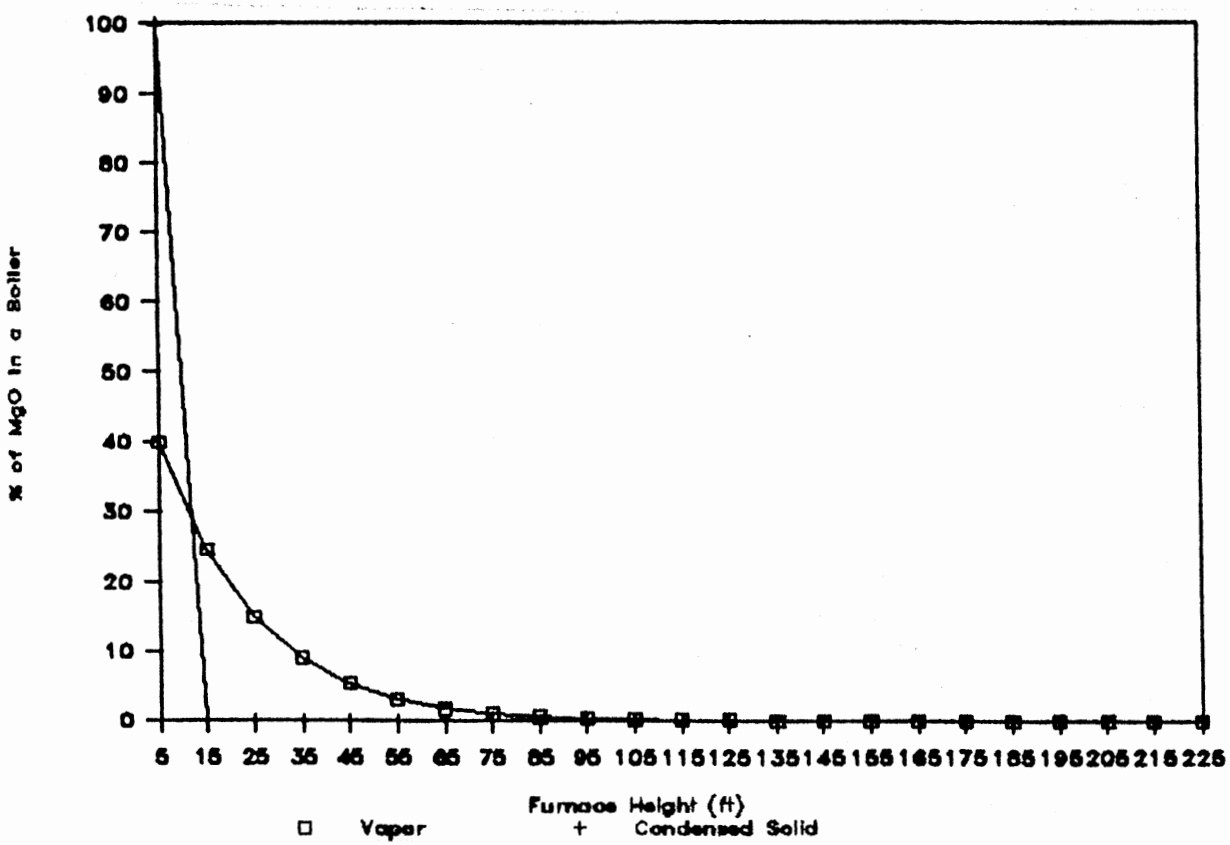


Figure 13. Distribution of MgO at Different Locations

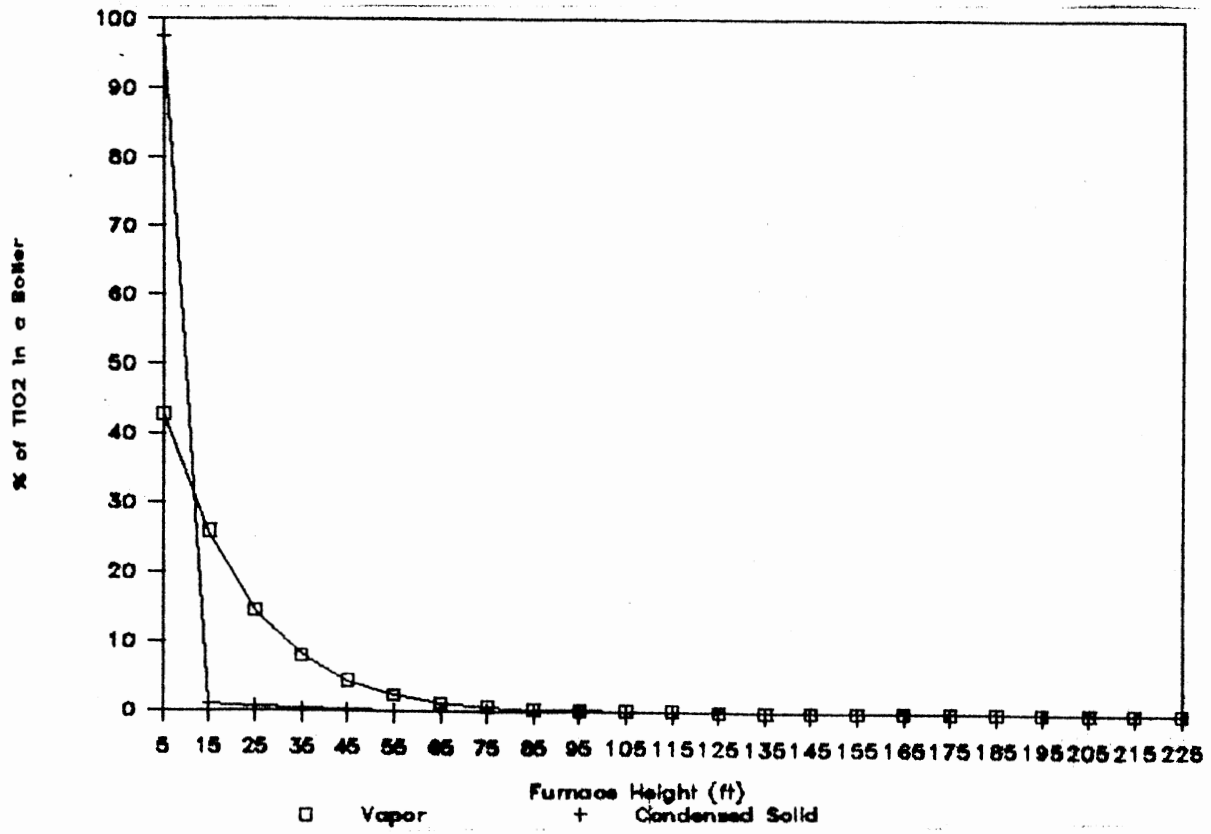


Figure 14. Distribution of TiO_2 at Different Locations

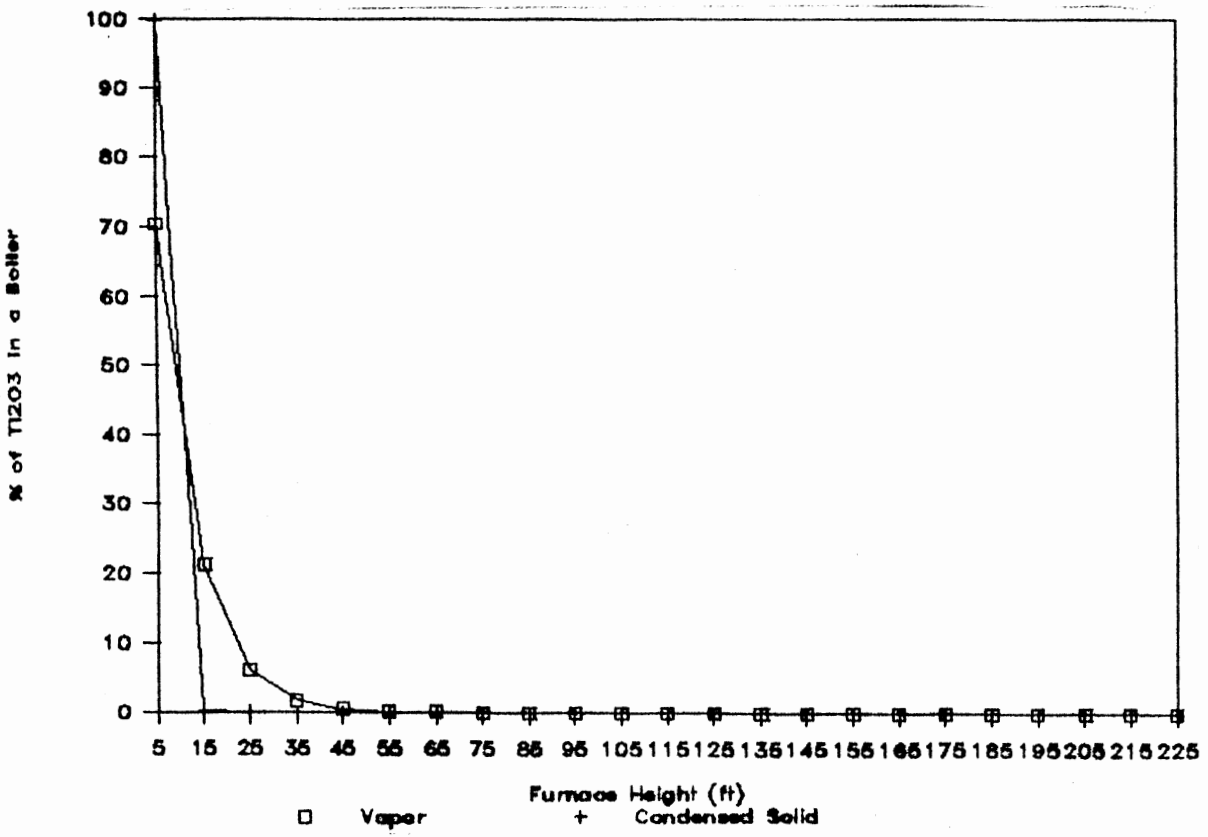


Figure 15. Distribution of Ti_2O_3 at Different Locations

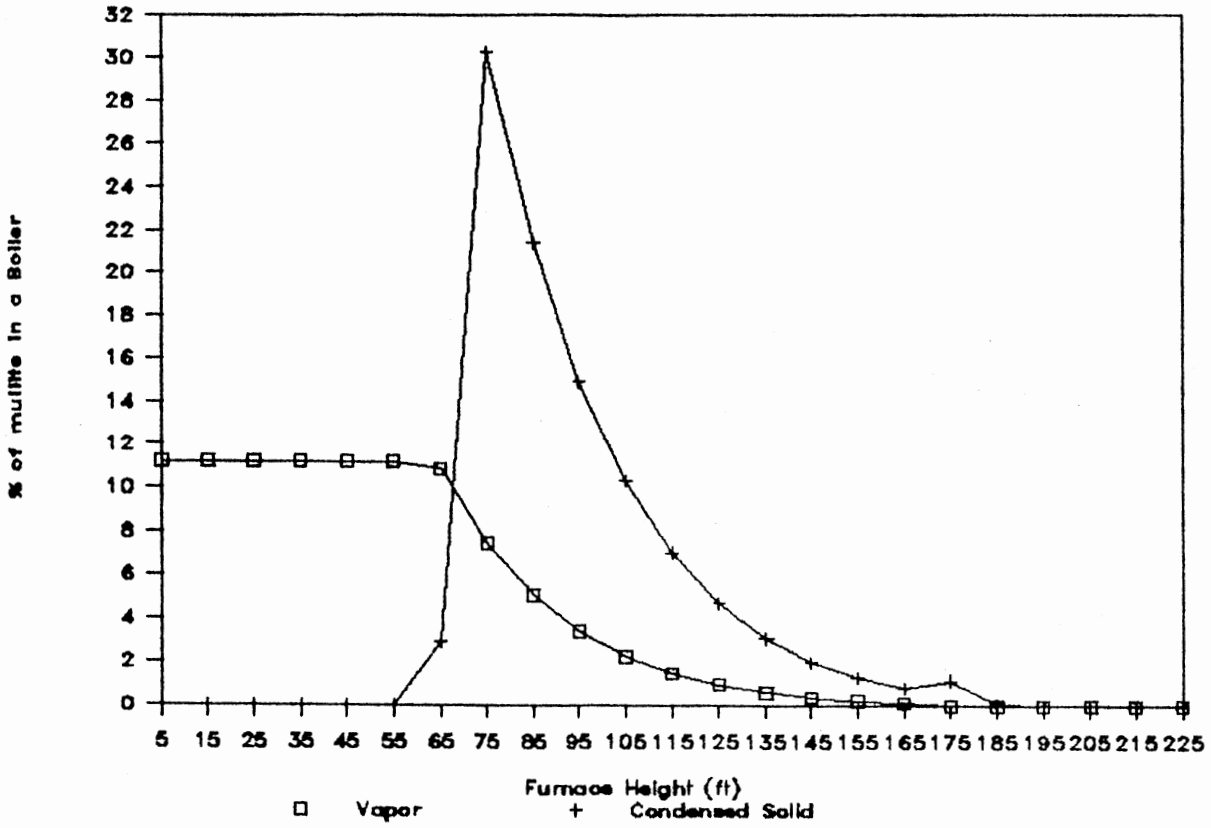


Figure 16. Distribution of $Al_6Si_2O_{13}$ at Different Locations

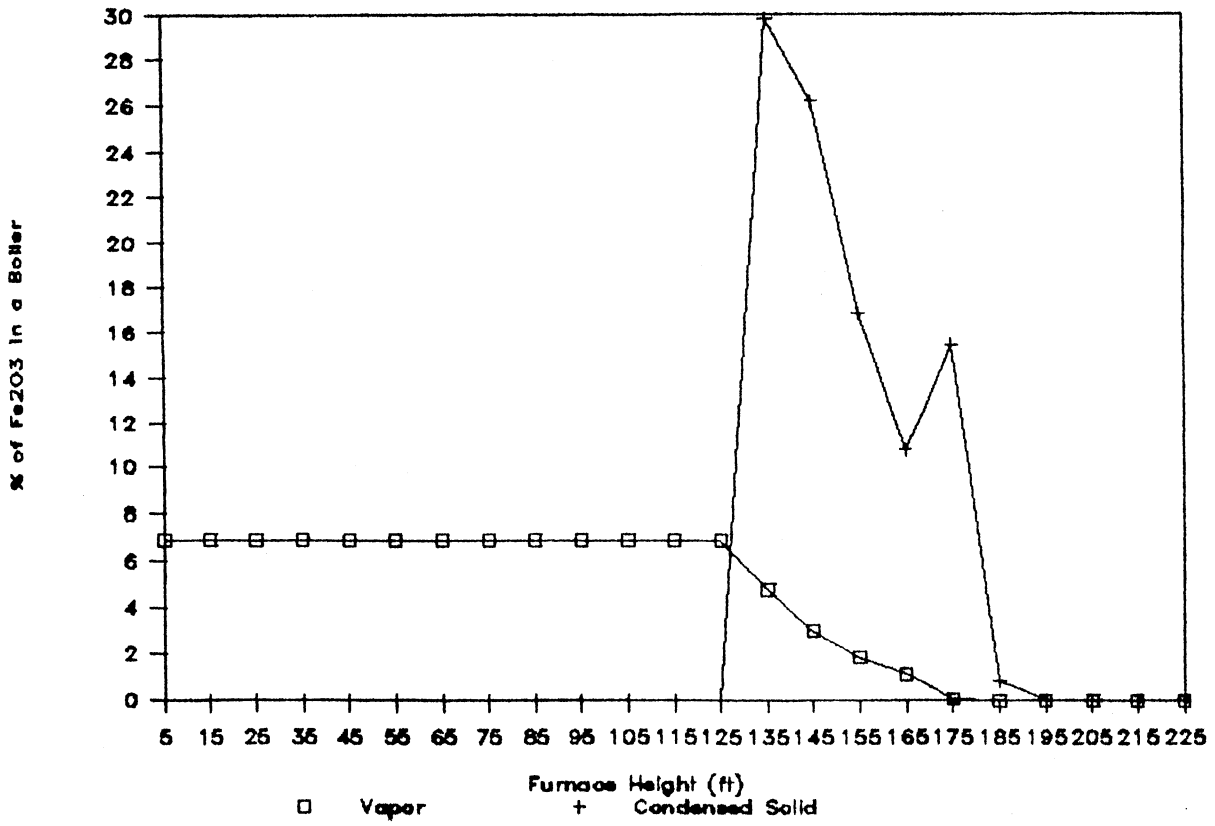


Figure 17. Distribution of Fe_2O_3 at Different Locations

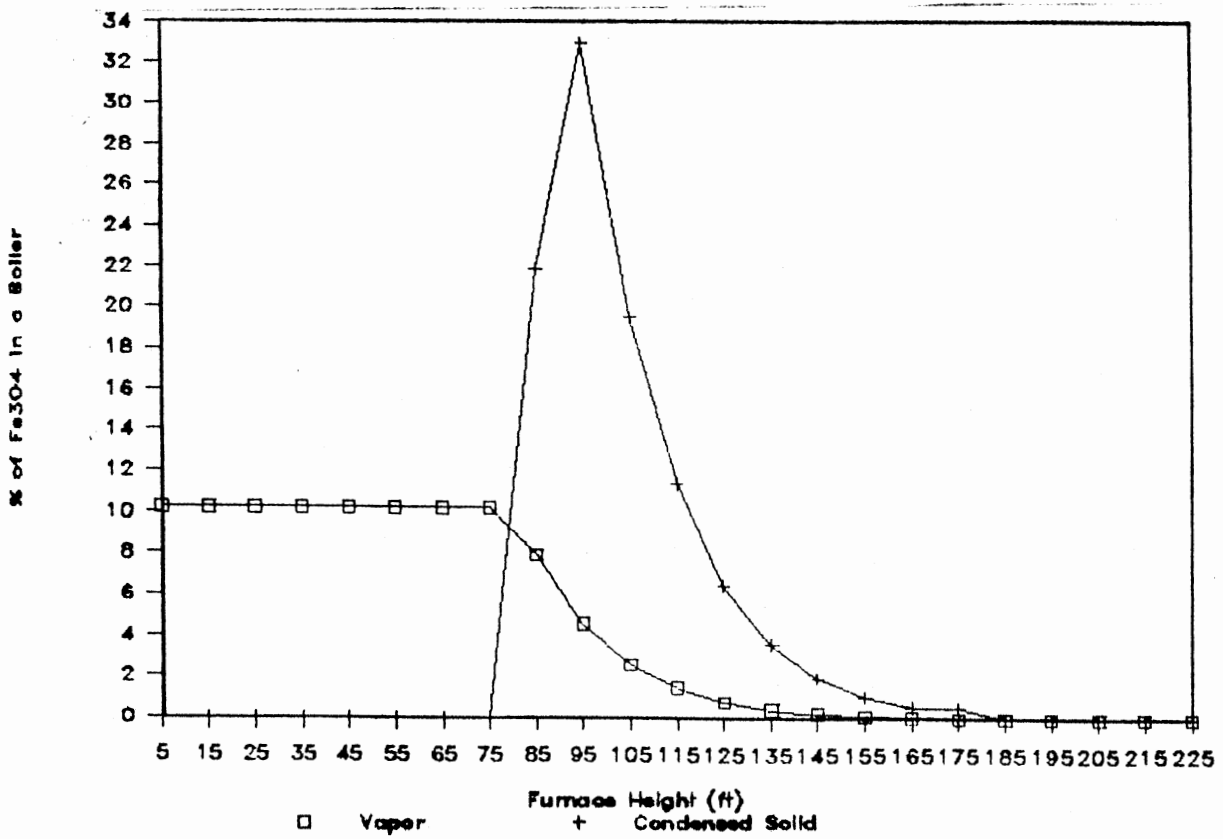


Figure 18. Distribution of Fe_3O_4 at Different Locations

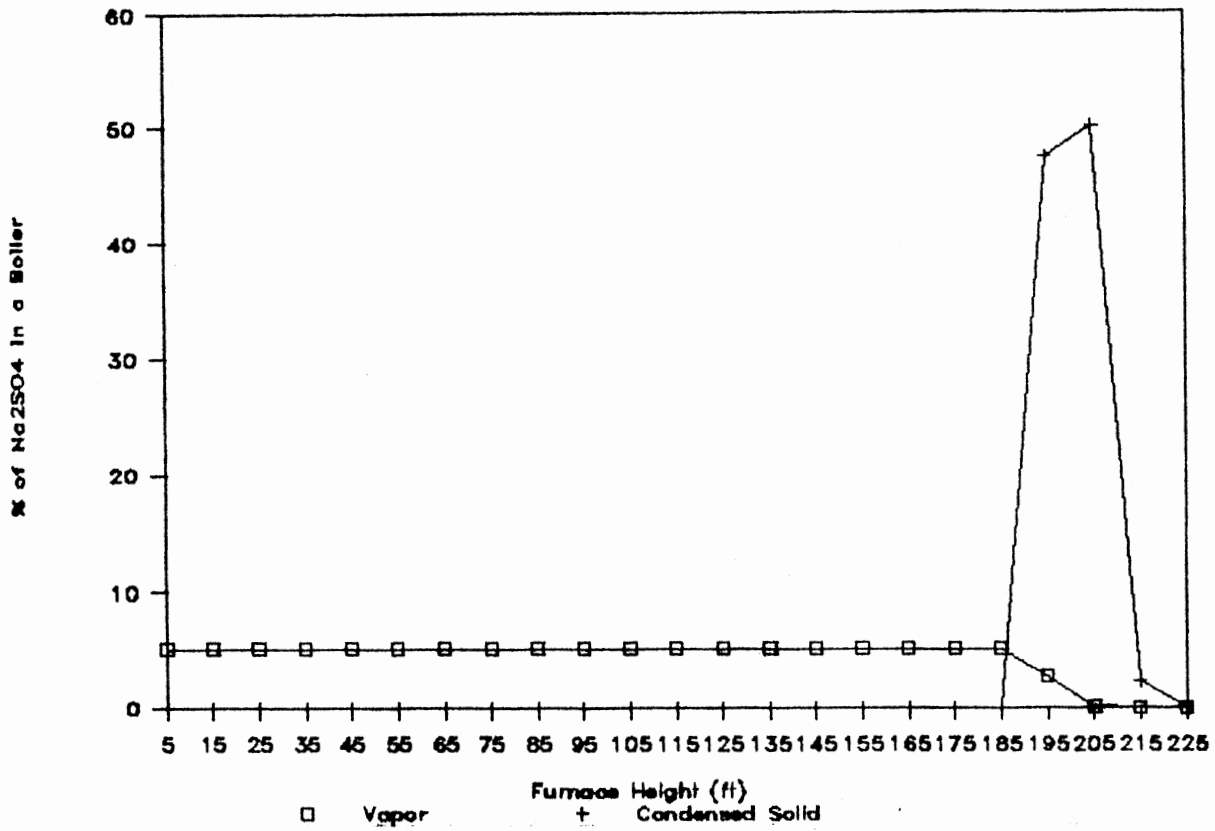


Figure 19. Distribution of Na_2SO_4 at Different Locations

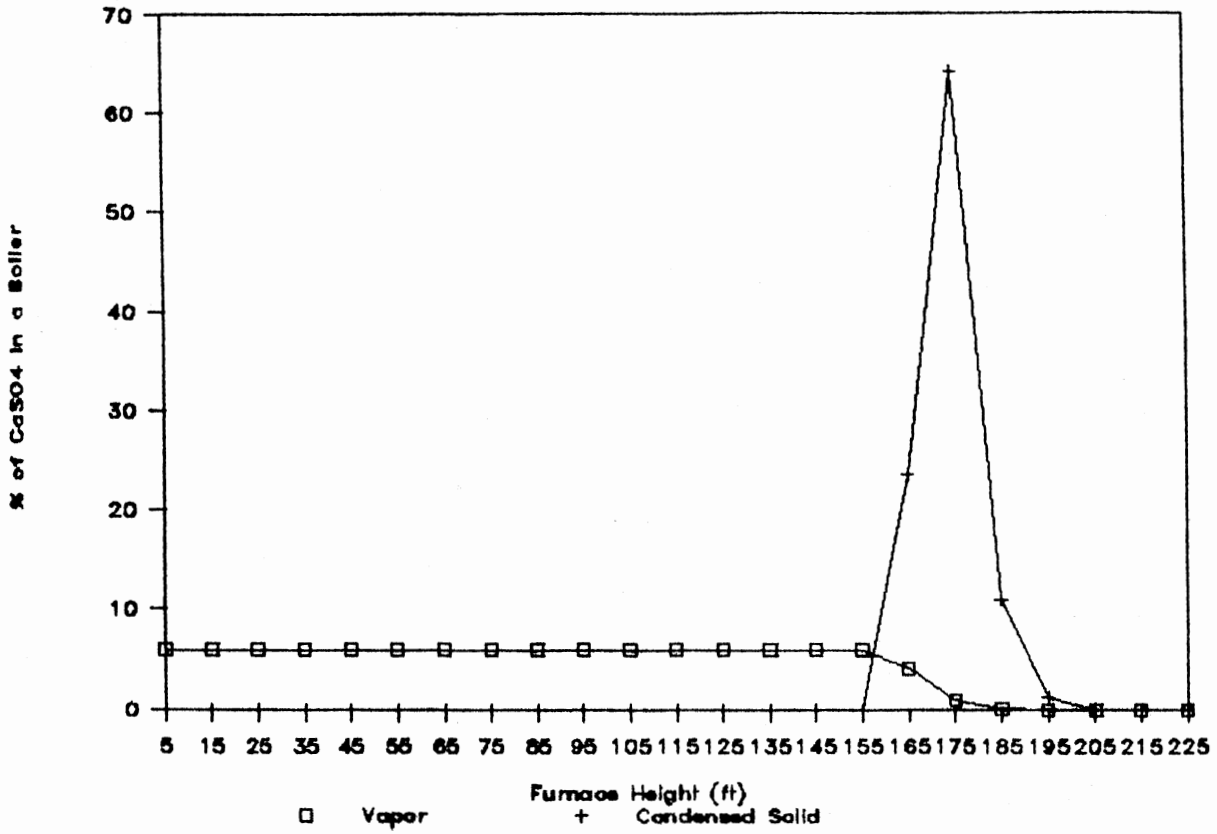


Figure 20. Distribution of $CaSO_4$ at Different Locations

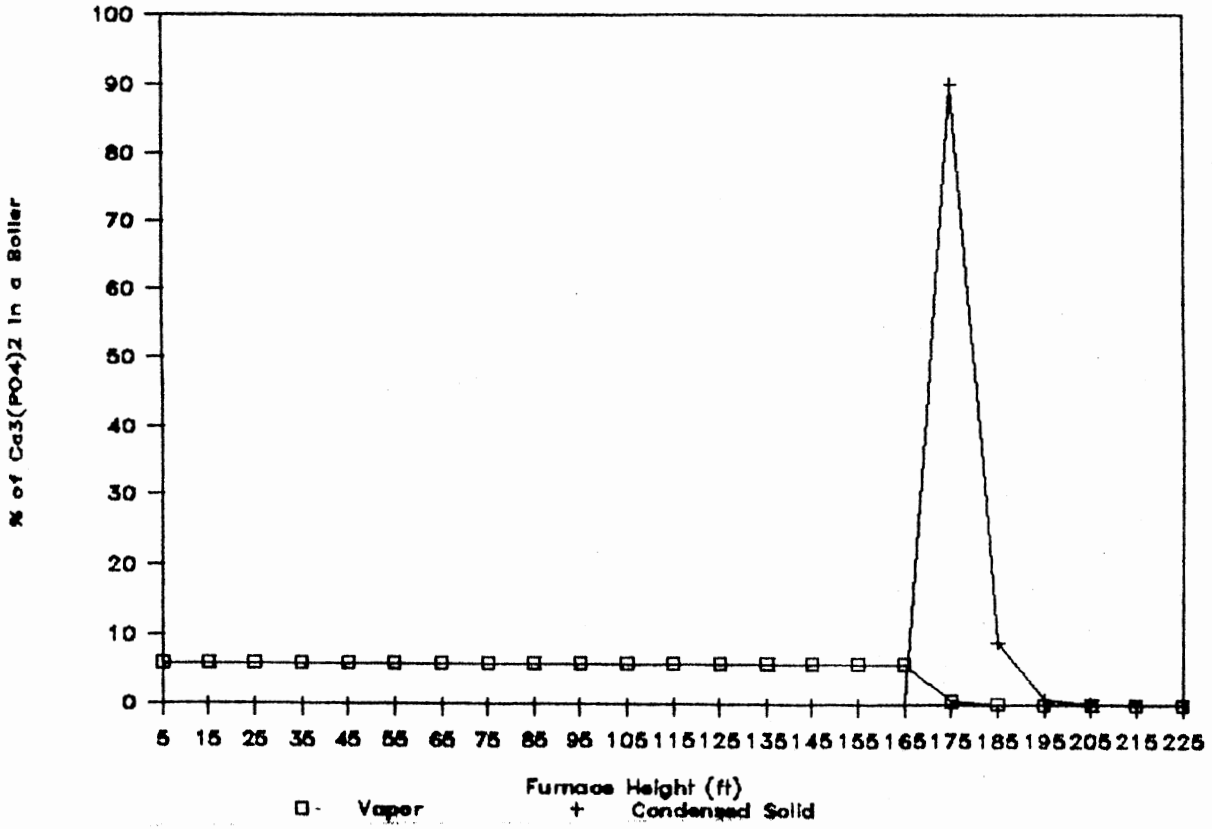


Figure 21. Distribution of $Ca_3(PO_4)_2$ at Different Locations

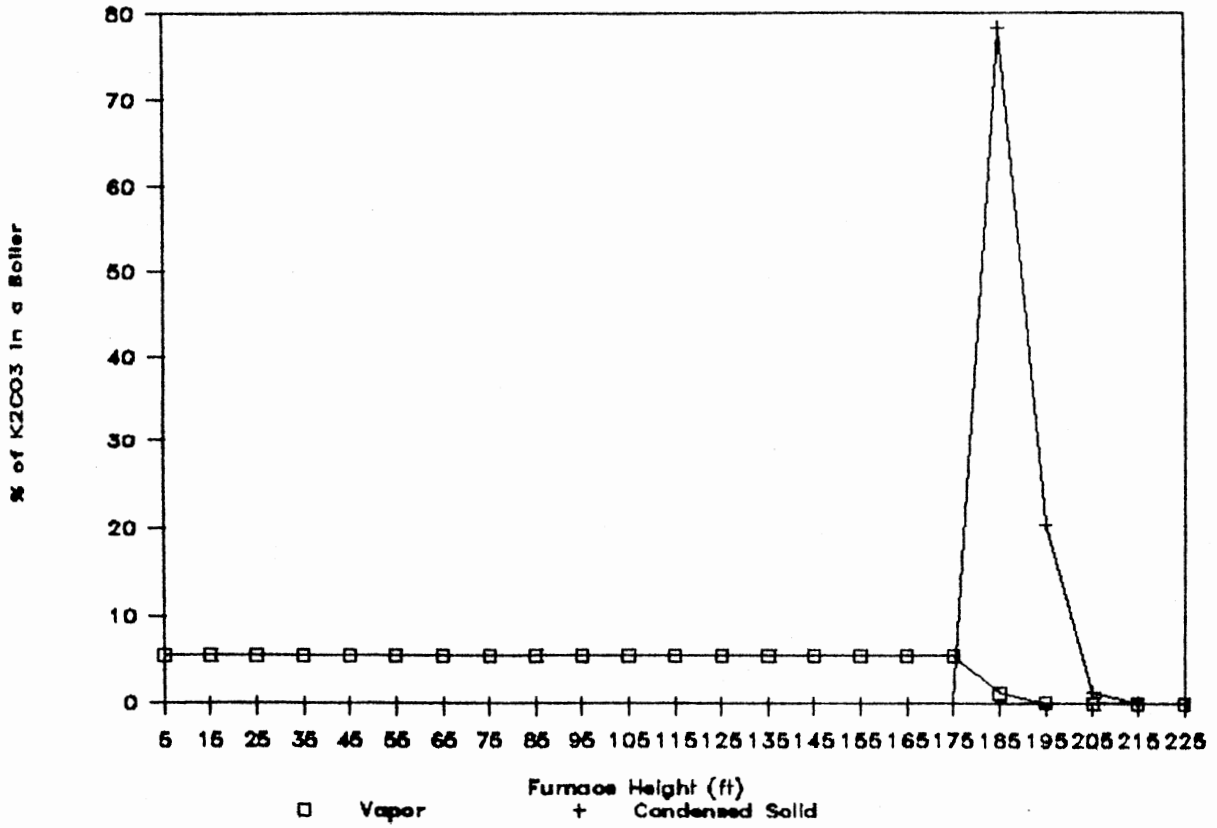


Figure 22. Distribution of K_2CO_3 at Different Locations

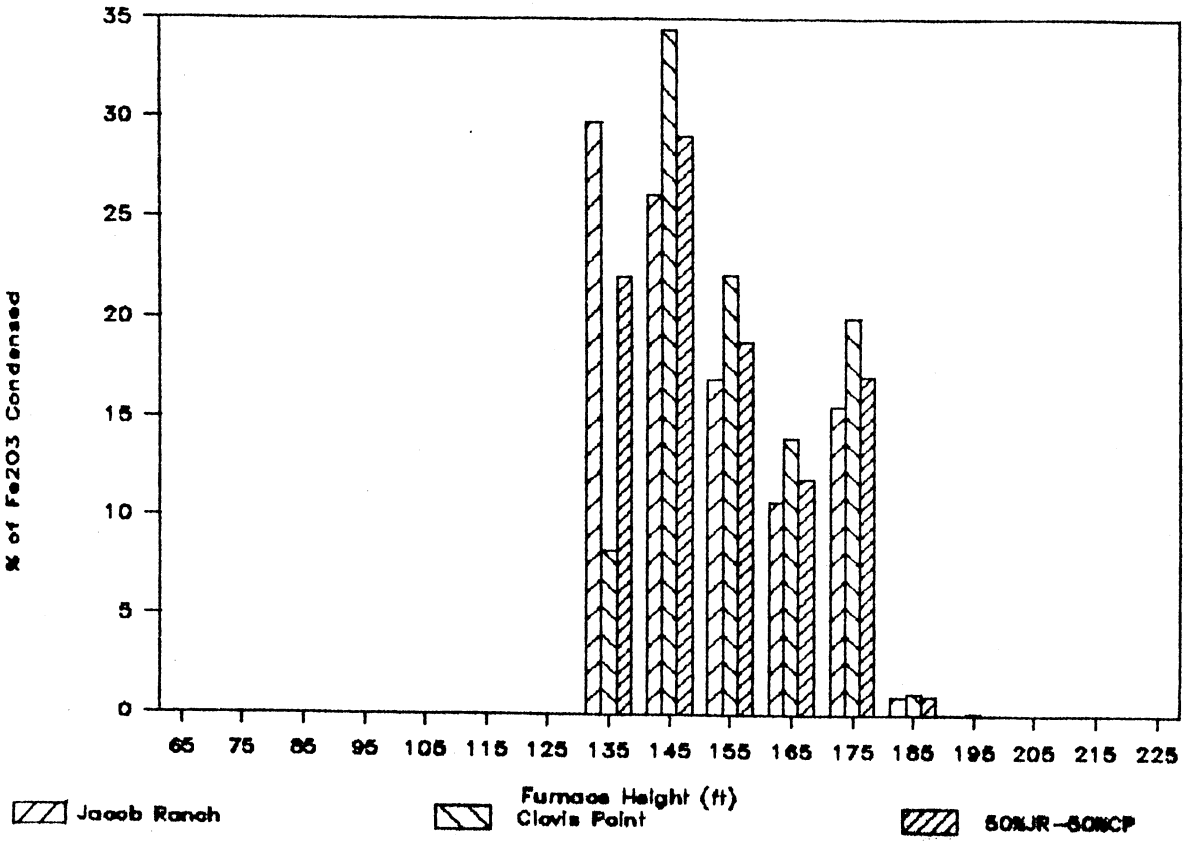


Figure 23. Percentage of Total Fe_2O_3 That Deposits at Different Locations in the Boiler for Coals and Their 50-50 Blend

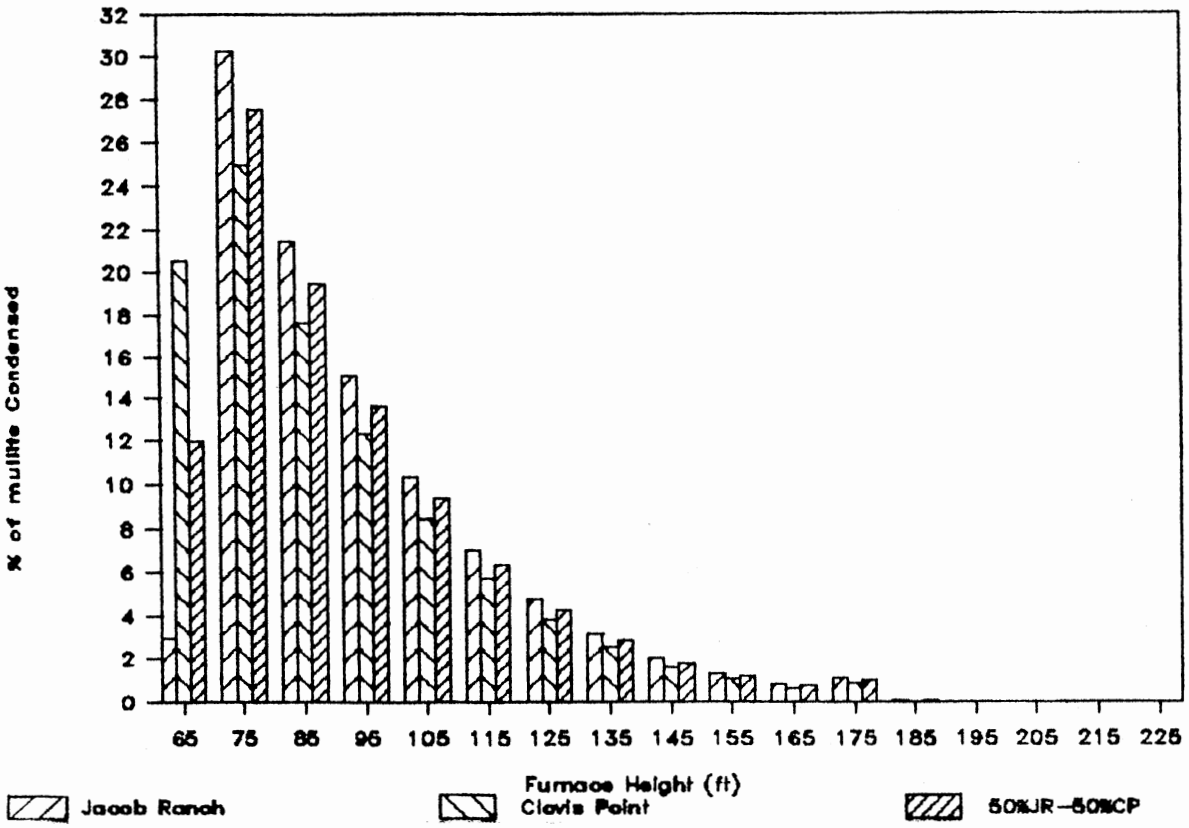


Figure 24. Percentage of Total Mullite That Deposits at Different Locations in the Boiler for Two Coals and Their 50-50 Blend

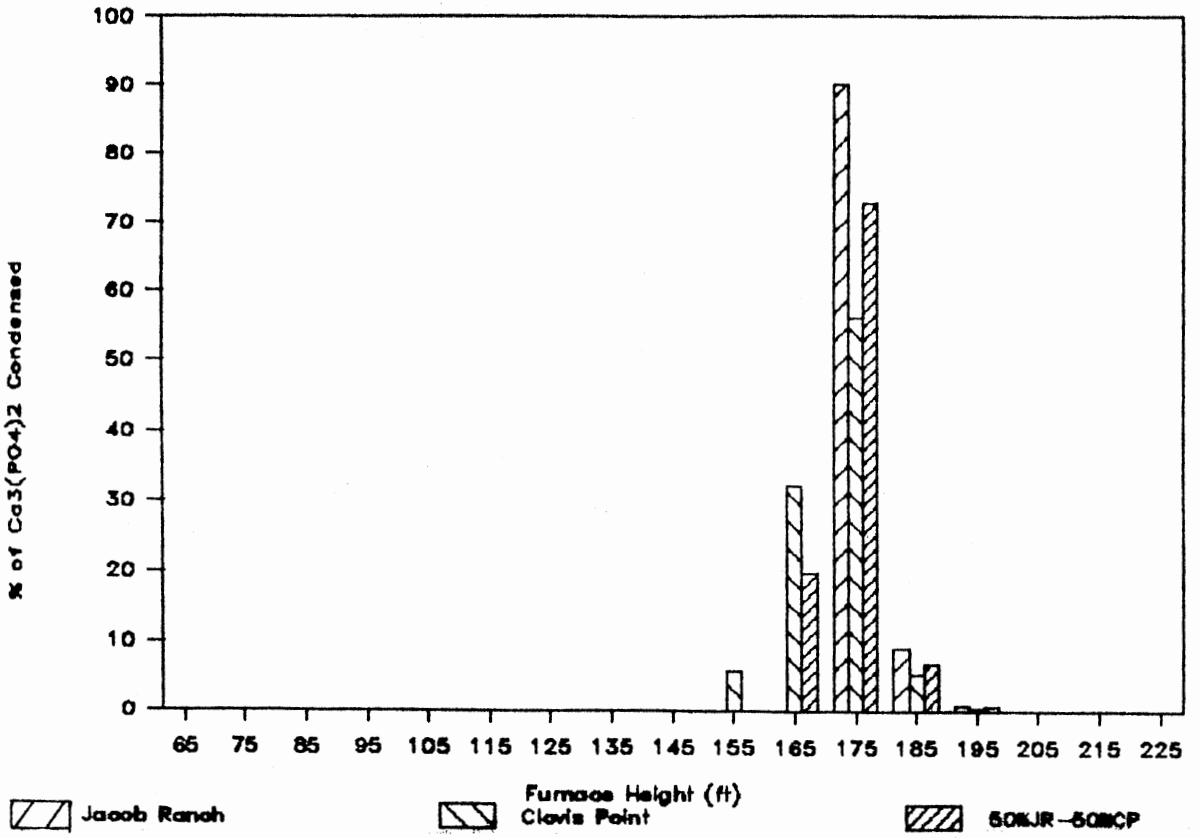


Figure 25. Percentage of Total $Ca_3(PO_4)_2$ That Deposits at Different Locations in the Boiler for Two Coals and Their 50-50 Blend

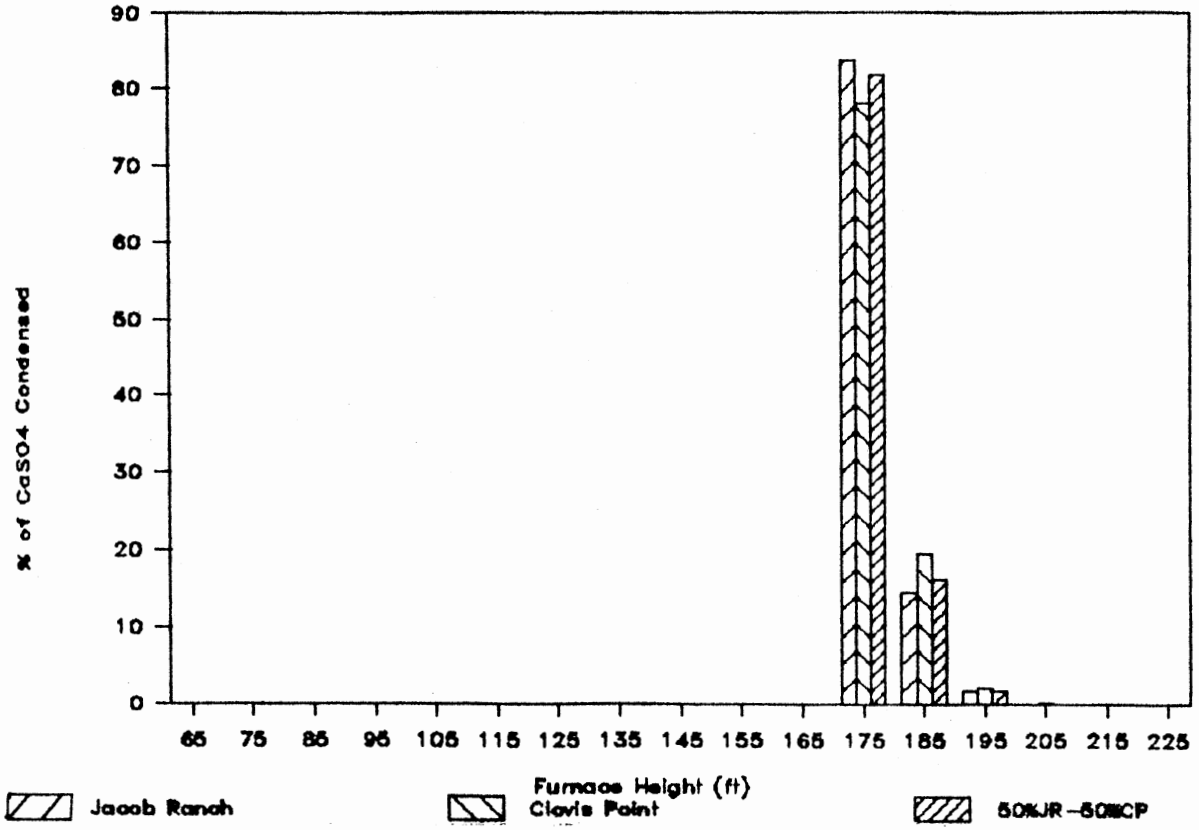


Figure 26. Percentage of Total $CaSO_4$ That Deposits at Different Locations in the Boiler for Two Coals and Their 50-50 Blend

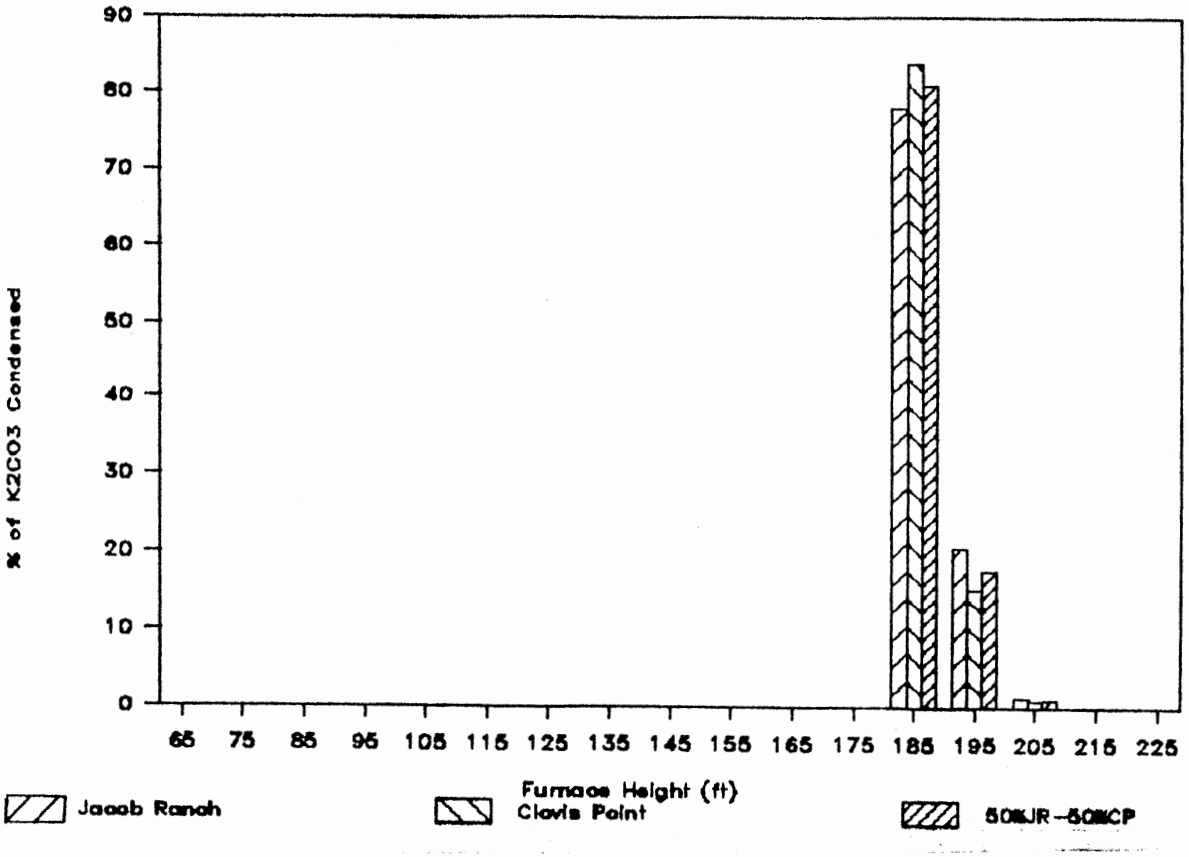


Figure 27. Percentage of Total K_2CO_3 That Deposits at Different Locations in the Boiler for Two Coals and Their 50-50 Blend

considered in analyzing this problem. A possible source of the problem could be major changes in the viscosity of the slag or its stickyness with only minor variation of composition.

For these two coal fuels, the solid deposition data are converted into the regular ash analysis form, and are shown in Tables XIV and XV as the wt % of oxides. The slagging flux at different locations are also listed in these tables. Figures 28 to 38 show the composition of ash deposits at different locations when Jacob Ranch coal is burned. These results can be compared with the samples removed from the PSO power plant in Oolagah, Oklahoma. Table XVI gives an analysis of a representative economizer deposit. Table XVII lists the analysis of a sample taken from the secondary superheat tubes. Table XVIII shows the analysis of slag removed when Clovis Point coal was burned and Table XIX shows the analysis of a slag removed when an unknown blend of Oklahoma coal and Clovis Point was burned.

The economizer is usually located in the 800 - 1000^{0} C region where deposits tend to have high sulfur content and significant amounts of phosphorus. In this model, the economizer is located between 175 - 195 ft, and the deposit also shows high contents of sulfur and significant amounts of phosphorus. This model assumes constant pressure and equilibrium condensation in each stage. Furthermore it does not consider any generation or transport of particles in these stages. However, in actual boilers, the draft force

TABLE XIV

JACOBS RANCH MINERAL WT % AT VARIOUS HEIGHTS

Height (ft)	T (K)	Fe as Fe_2O_3	Ca as CaO	Mg as MgO	Na as Na_2O	K as K_2O	Si as SiO_2	Al as Al_2O_3	Ti as TiO_2	P as P_2O_5	S as SO_3	Slagging flux $kg/h \cdot m^2$	Contribution as percent of ash in the coal
*	1958	0.00	26.83	12.60	0.00	0.00	37.27	22.76	1.54	0.00	0.00	87.98	37.29
15	1928	0.00	0.03	0.09	0.00	0.00	99.44	0.26	0.18	0.00	0.00	22.22	9.42
25	1899	0.00	0.03	0.10	0.00	0.00	99.48	0.26	0.13	0.00	0.00	14.14	5.99
35	1870	0.00	0.03	0.10	0.00	0.00	99.51	0.25	0.11	0.00	0.00	8.88	3.76
45	1840	0.00	0.03	0.10	0.00	0.00	99.53	0.25	0.09	0.00	0.00	5.49	2.33
55	1811	0.00	0.03	0.10	0.00	0.00	99.55	0.25	0.08	0.00	0.00	3.34	1.42
65	1781	0.00	0.02	0.09	0.00	0.00	93.64	6.18	0.07	0.00	0.00	3.28	1.39
75	1752	0.00	0.01	0.04	0.00	0.00	56.74	43.18	0.03	0.00	0.00	13.65	5.79
85	1722	0.00	0.01	0.03	0.00	0.00	53.34	46.60	0.02	0.00	0.00	9.51	4.03
95	1693	0.00	0.01	0.03	0.00	0.00	50.02	49.93	0.02	0.00	0.00	6.56	2.78
105	1663	39.58	0.00	0.02	0.00	0.00	28.31	32.08	0.01	0.00	0.00	6.46	2.74
115	1634	60.61	0.00	0.01	0.00	0.00	17.30	22.08	0.00	0.00	0.00	6.02	2.55
125	1605	58.33	0.00	0.01	0.00	0.00	17.18	24.48	0.00	0.00	0.00	3.75	1.59
135	1575	81.86	0.00	0.00	0.00	0.00	7.05	11.09	0.00	0.00	0.00	4.15	1.76
145	1546	84.94	0.00	0.00	0.00	0.00	5.54	9.52	0.00	0.00	0.00	3.01	1.28
155	1516	85.05	0.00	0.00	0.00	0.00	5.23	9.72	0.00	0.00	0.00	1.88	0.80
165	1487	85.15	0.00	0.00	0.00	0.00	4.97	9.88	0.00	0.00	0.00	1.16	0.49
175	1337	4.99	37.86	0.00	0.00	0.00	0.27	0.59	0.00	5.18	51.12	22.12	9.38
185	1210	0.90	22.39	0.00	0.00	43.79	0.04	0.11	0.00	1.83	30.94	6.67	2.83
195	1083	0.09	5.37	0.00	27.27	24.21	0.00	0.01	0.00	0.33	42.70	2.83	1.12
205	956	0.00	0.52	0.00	42.14	2.15	0.00	0.00	0.00	0.02	55.15	1.75	0.74
215	829	0.00	0.37	0.00	42.65	1.36	0.00	0.00	0.00	0.01	55.60	0.08	0.03
225	701	0.00	0.24	0.00	43.07	0.74	0.00	0.00	0.00	0.00	55.95	0.001	4.24×10^{-4}
Fly Ash	-	0.00	0.00	0.00	99.01	0.00	0.00	0.00	0.00	0.00	0.99	0.21**	4.80×10^{-4}

* Residual ash that falls to the bottom of the furnace and the slag that is formed in the first stage.

** The rate of fly ash leaving the boiler (kg/h)

TABLE XV

CLOVIS PLANT MINERAL WT % AT VARIOUS HEIGHTS

Height (ft)	T (K)	Fe as Fe_2O_3	Ca as CaO	Mg as MgO	Na as Na_2O	K as K_2O	Si as SiO_2	Al as Al_2O_3	Ti as TiO_2	P as P_2O_5	S as SO_3	Slagging flux $kg/h \cdot m^2$	Contribution as percent of ash in the coal
*	1937	0.00	22.94	9.36	0.00	0.00	50.71	16.03	0.97	0.00	0.00	102.56	48.51
15	1908	0.00	0.03	0.10	0.00	0.00	99.47	0.26	0.14	0.00	0.00	14.69	6.95
25	1879	0.00	0.03	0.10	0.00	0.00	99.51	0.26	0.11	0.00	0.00	9.30	4.40
35	1850	0.00	0.03	0.10	0.00	0.00	99.53	0.25	0.09	0.00	0.00	5.81	2.75
45	1820	0.00	0.03	0.10	0.00	0.00	99.55	0.25	0.08	0.00	0.00	3.57	1.69
55	1791	0.00	0.03	0.10	0.00	0.00	99.56	0.24	0.07	0.00	0.00	2.16	1.02
65	1762	0.00	0.01	0.05	0.00	0.00	67.28	32.62	0.04	0.00	0.00	8.81	4.17
75	1733	0.00	0.01	0.04	0.00	0.00	54.55	45.38	0.02	0.00	0.00	9.84	4.65
85	1704	0.00	0.01	0.03	0.00	0.00	51.23	48.71	0.02	0.00	0.00	6.84	3.24
95	1675	0.00	0.01	0.03	0.00	0.00	48.04	51.91	0.01	0.00	0.00	4.70	2.22
105	1646	11.78	0.00	0.02	0.00	0.00	39.73	48.45	0.01	0.00	0.00	3.48	1.65
115	1617	59.28	0.00	0.01	0.00	0.00	17.21	23.49	0.00	0.00	0.00	4.12	1.95
125	1587	56.83	0.00	0.01	0.00	0.00	17.18	25.98	0.00	0.00	0.00	2.57	1.22
135	1558	65.35	0.00	0.00	0.00	0.00	13.03	21.62	0.00	0.00	0.00	1.86	0.88
145	1529	85.01	0.00	0.00	0.00	0.00	5.35	9.64	0.00	0.00	0.00	2.10	0.99
155	1500	75.63	3.15	0.00	0.00	0.00	4.51	8.72	0.00	7.98	0.00	1.70	0.80
165	1471	40.43	14.89	0.00	0.00	0.00	2.30	4.72	0.00	37.66	0.00	2.92	1.38
175	1323	6.35	36.77	0.00	0.00	0.00	0.34	0.75	0.00	7.58	48.21	12.85	6.08
185	1197	0.71	19.13	0.00	0.00	50.07	0.03	0.08	0.00	1.52	26.46	5.83	2.76
195	1071	0.04	2.33	0.00	36.60	10.40	0.00	0.00	0.00	0.14	50.50	4.41	2.09
205	946	0.00	0.51	0.00	42.19	2.08	0.00	0.00	0.00	0.02	55.20	1.25	0.5
215	820	0.00	0.36	0.00	42.69	1.30	0.00	0.00	0.00	0.01	55.64	0.05	0.02
225	694	0.00	0.23	0.00	43.09	0.71	0.00	0.00	0.00	0.00	55.97	3×10^{-5}	1.42×10^{-5}
Fly Ash	-	0.00	0.00	0.00	99.03	0.01	0.00	0.00	0.00	0.00	0.97	0.014**	3.31×10^{-5}

* Residual ash that falls to the bottom of the furnace and the slag that is formed in the first stage.

** The rate of fly ash leaving the boiler (kg/h)

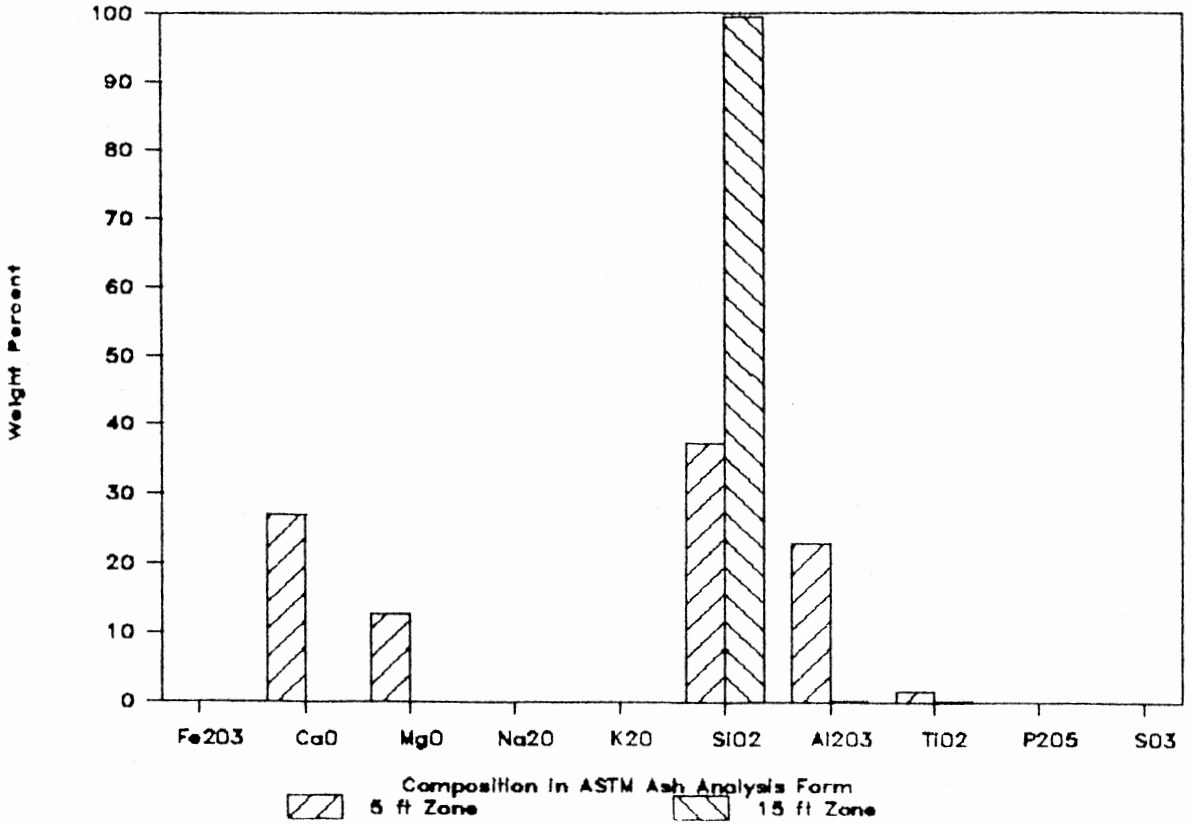


Figure 28. Composition of Ash Deposits at 5 ft and 15 ft Locations

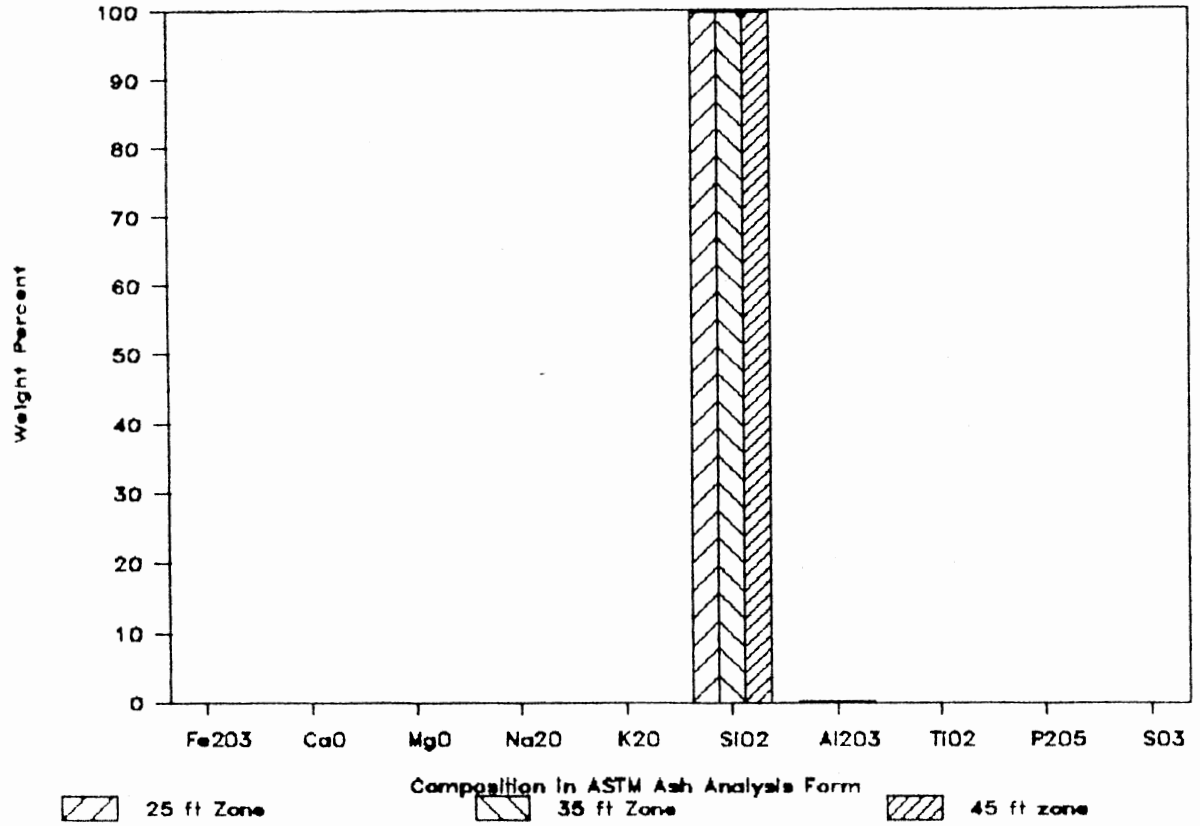


Figure 29. Composition of Ash Deposits at 25 ft, 35 ft and 45 ft Locations

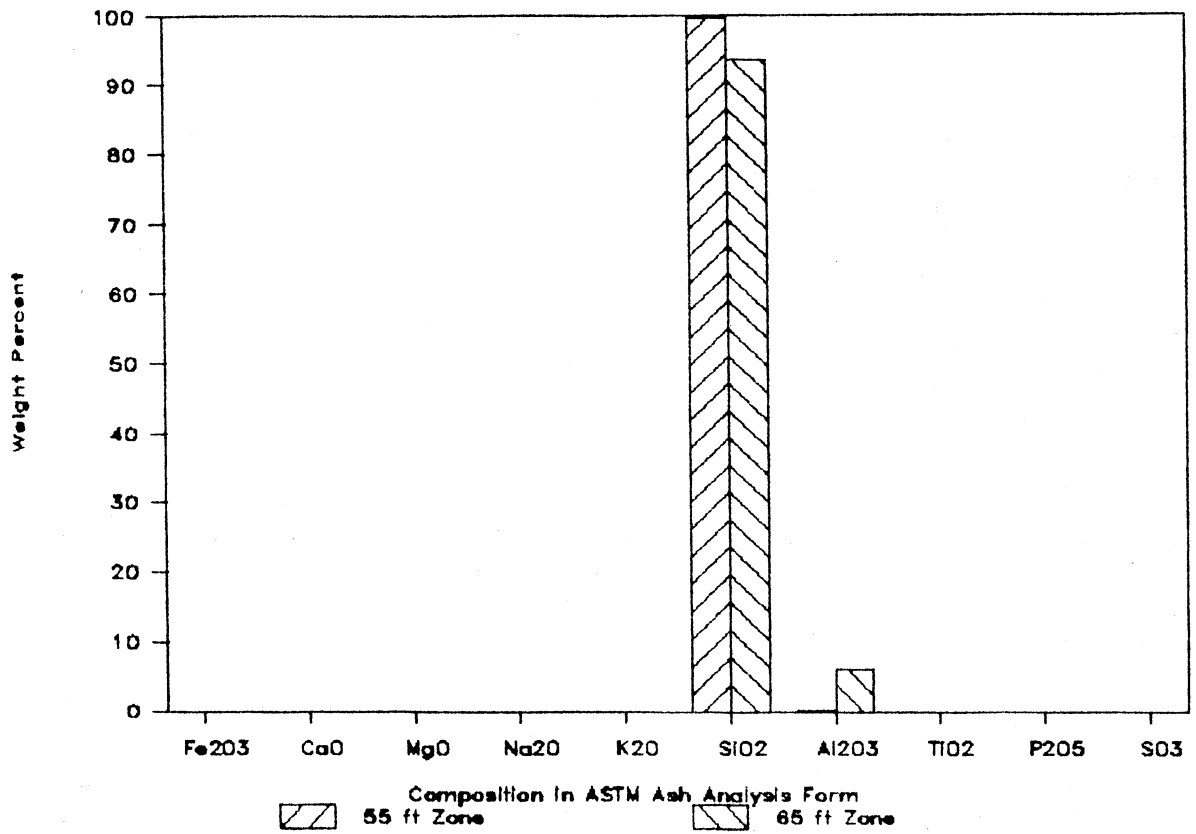


Figure 30. Composition of Ash Deposits at 55 ft and 65 ft Locations

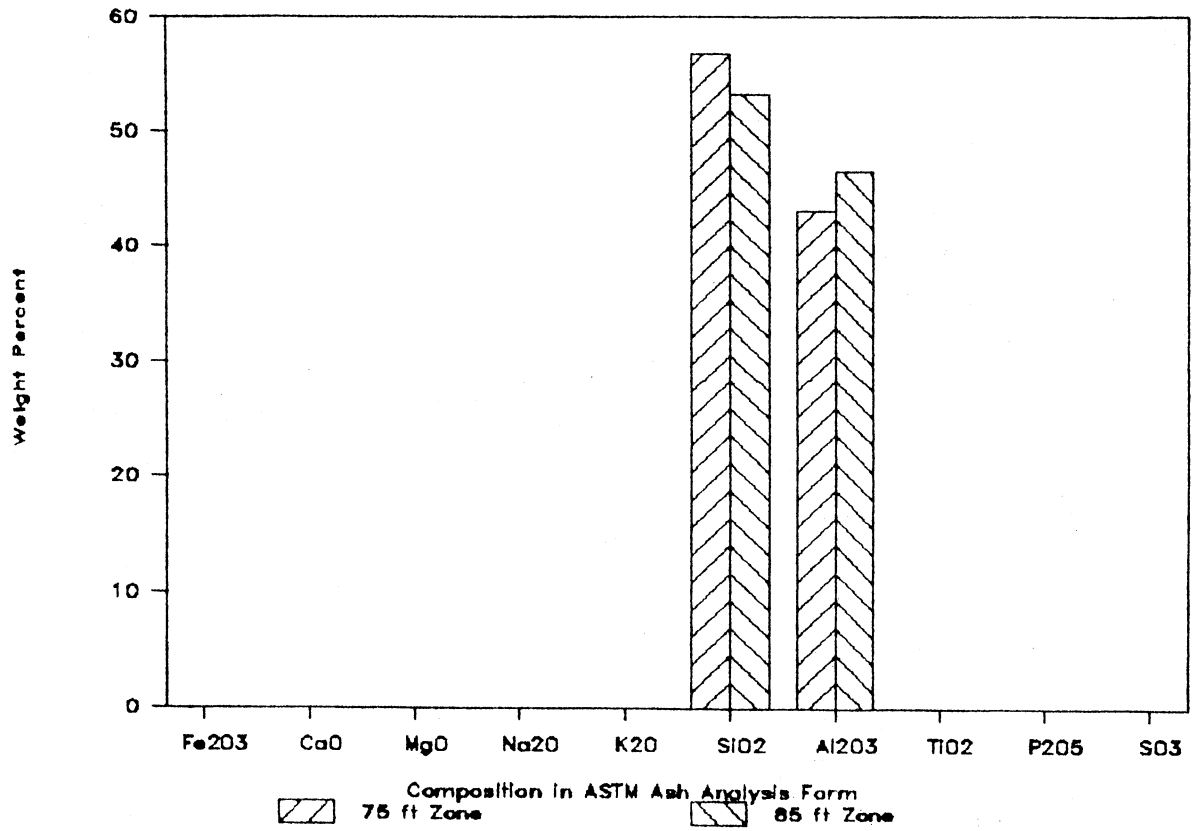


Figure 31. Composition of Ash Deposits at 75 ft and 85 ft Locations

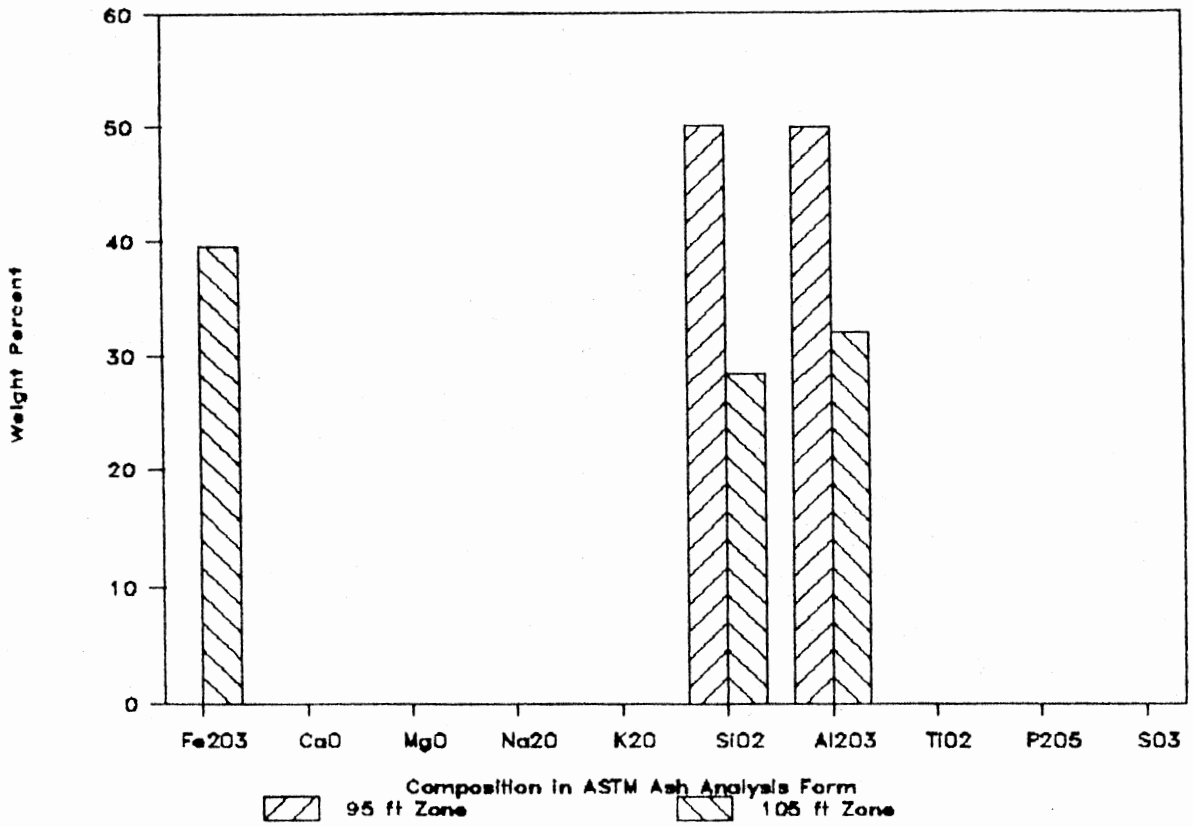


Figure 32. Composition of Ash Deposits at 95 ft and 105 ft Locations

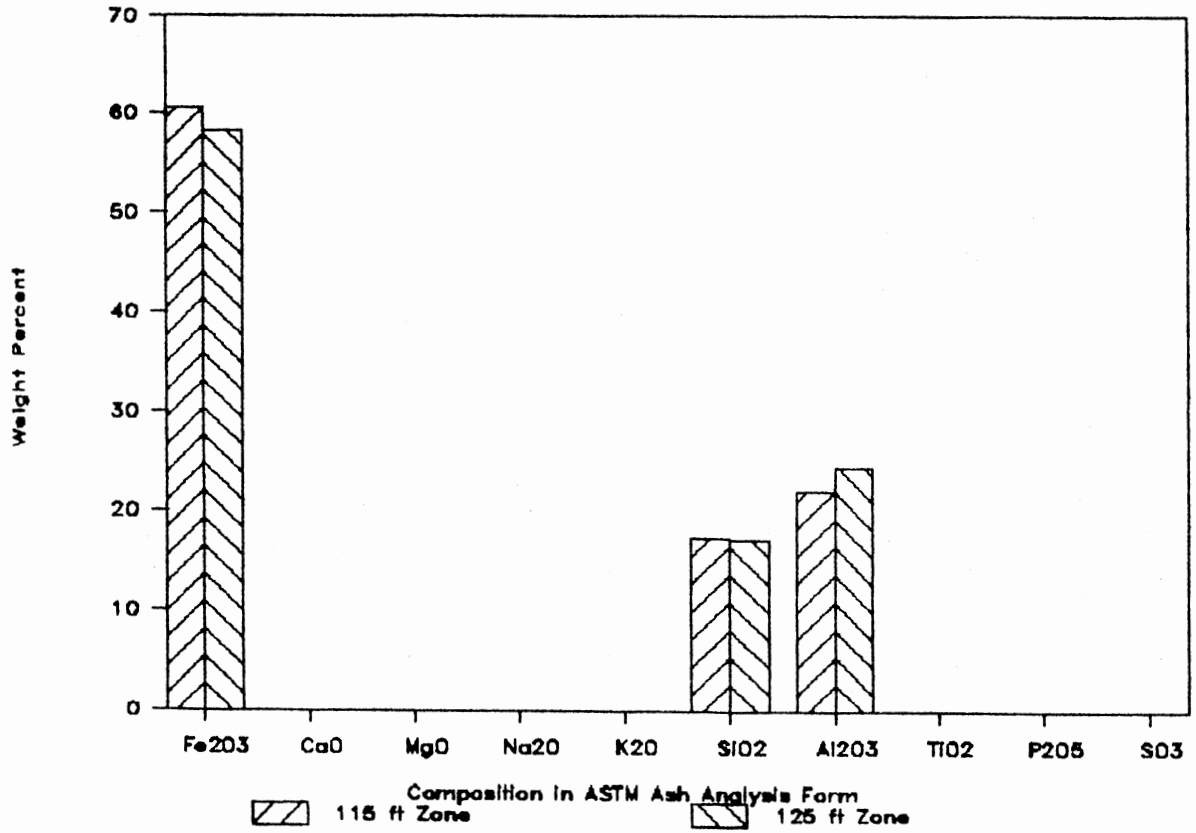


Figure 33. Composition of Ash Deposits at 115 ft and 125 ft Locations

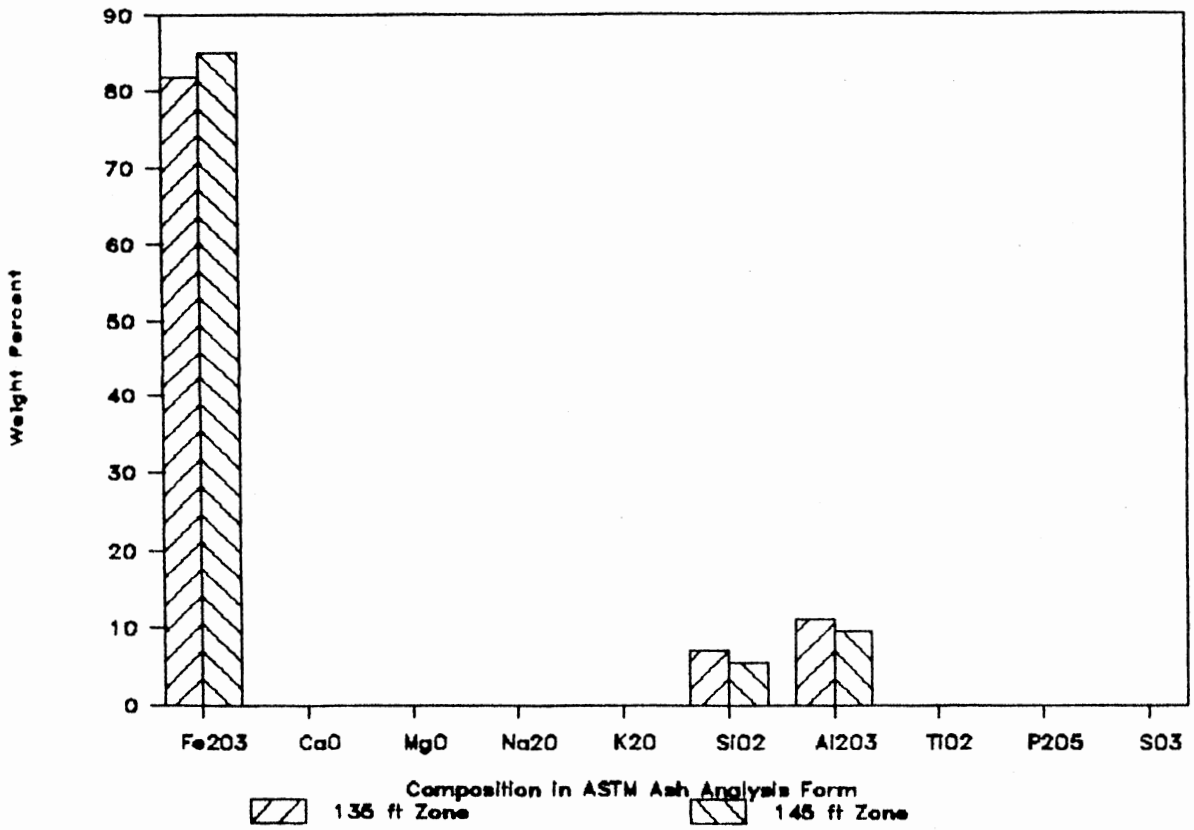


Figure 34. Composition of Ash Deposits at 135 ft and 145 ft Locations

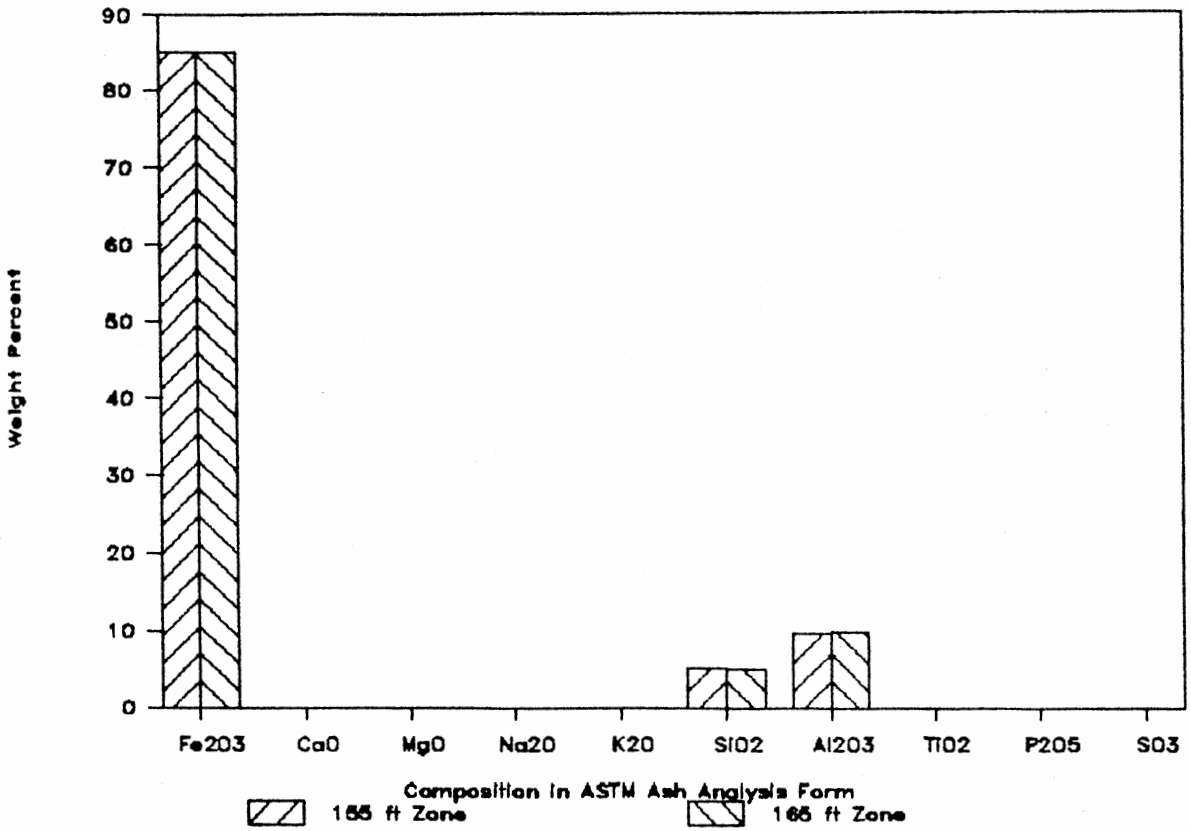


Figure 35. Composition of Ash Deposits at 155 ft and 165 ft Locations

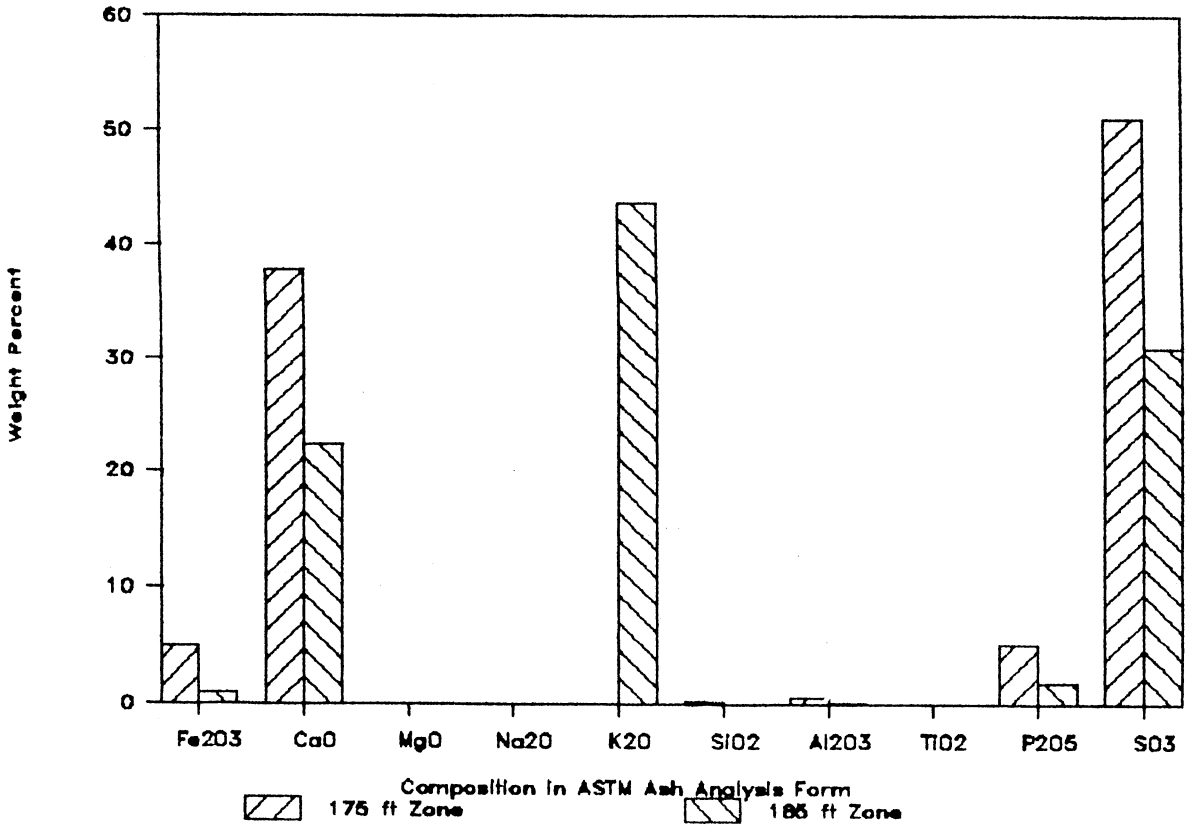


Figure 36. Composition of Ash Deposits at 175 ft and 185 ft Locations

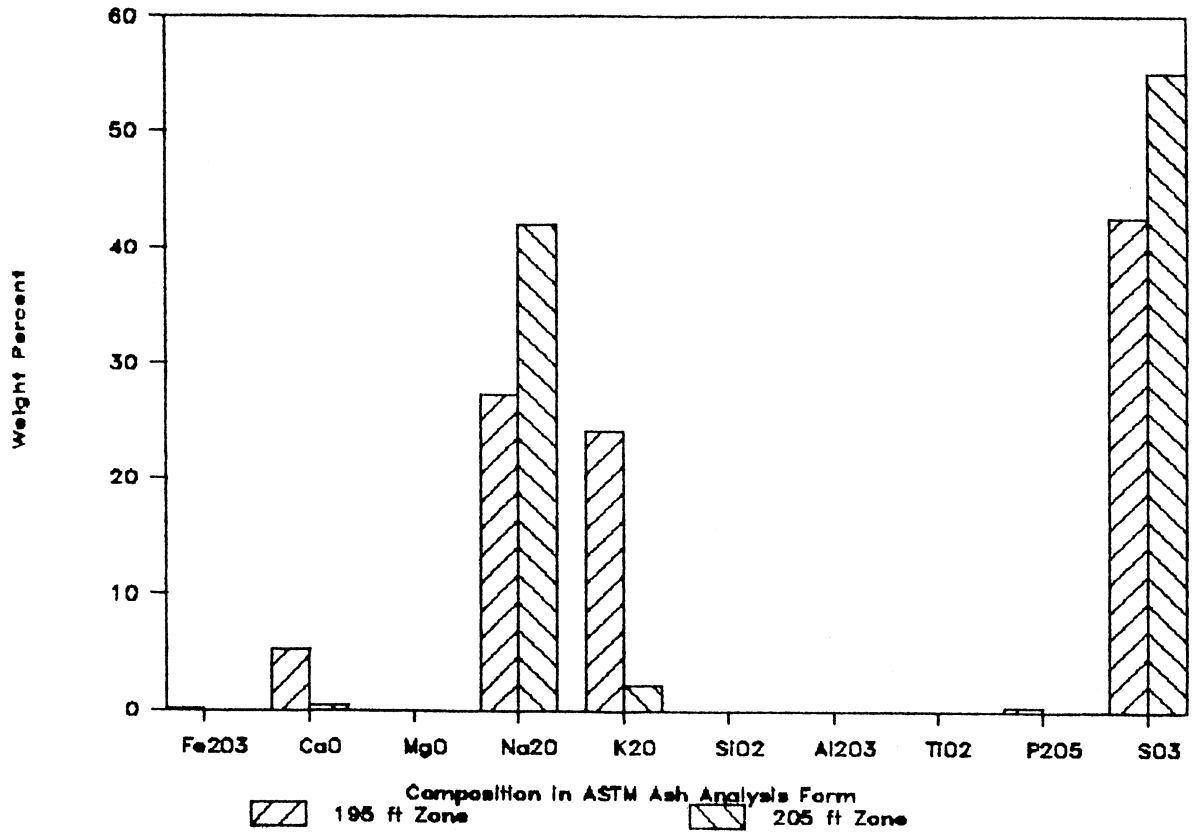


Figure 37. Composition of Ash Deposits at 195 ft and 205 ft Locations

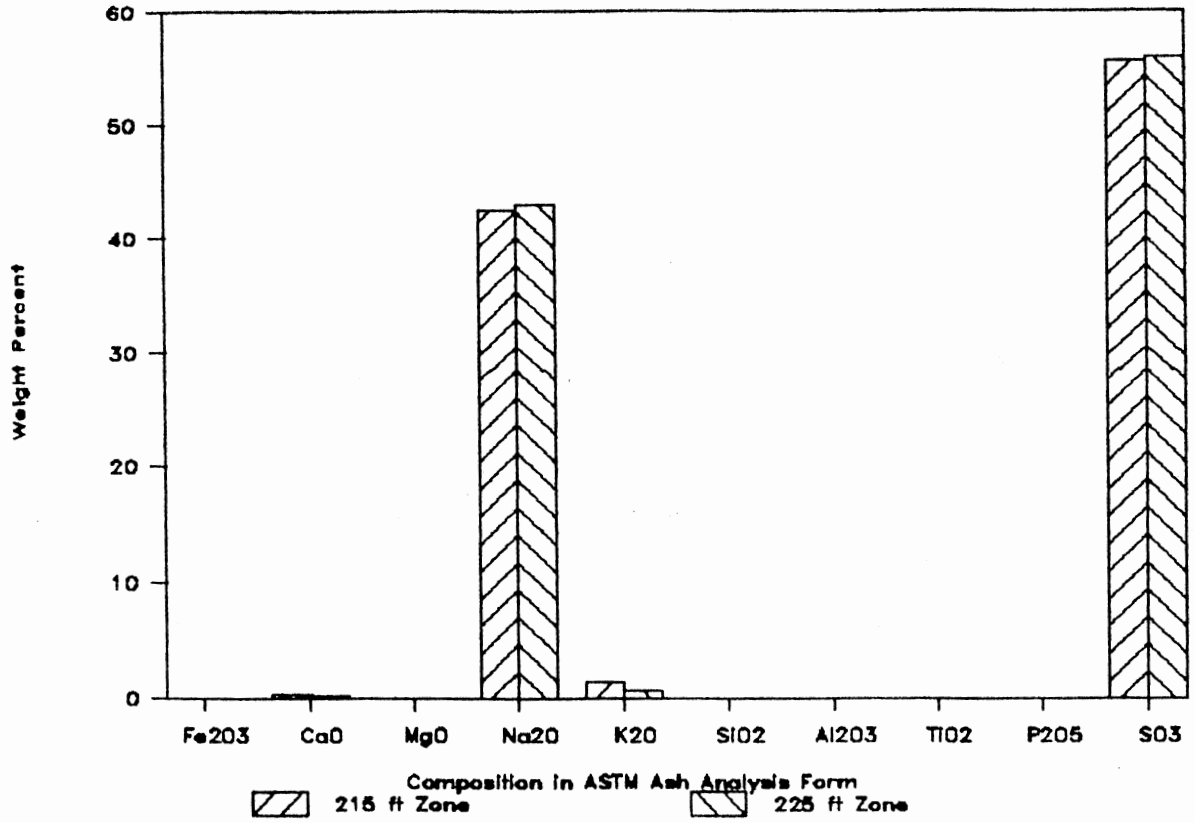


Figure 38. Composition of Ash Deposits at 215 ft and 225 ft Locations

TABLE XVI

PSO ECONOMIZER DEPOSIT COMPOSITION

Mineral analysis (Wt. %)	Light Layer	Dark Layer
Iron as Fe_2O_3	7.0	7.0
Calcium as CaO	21.0	20.0
Magnesium as MgO	5.0	5.0
Sodium as Na_2O	<1.0	1.0
Potassium as K_2O	<1.0	<1.0
Silicon as SiO_2	31.0	23.0
Aluminum as Al_2O_3	16.0	11.0
Titanium as TiO_2	1.0	1.0
Phosphorus as P_2O_5	4.0	4.0
Sulfur as SO_3	11.0	23.0

Data from Calgon Corporation

TABLE XVII

PSO SECONDARY SUPERHEATER DEPOSIT COMPOSITION

Source of Deposit	Secondary Superheater		
Temperature Range	1200 - 1400^{0}C		
Type of Deposit	Hard Scale		
Subdivisions	inner layer	middle layer	outer layer
Mineral Analysis Wt.%			
Iron as(Fe_2O_3)	5.29	5.61	5.55
Calcium as (CaO)	16.86	27.81	18.20
Magnesium as (MgO)	2.70	3.29	2.99
Sodium as (Na_2O)	0.63	0.55	0.56
Potassium as (K_2O)	1.11	0.94	0.86
Silicon as (SiO_2)	48.46	47.08	46.22
Aluminum as (Al_2O_3)	19.58	18.98	18.98
Titanium as (TiO_2)	0.93	1.09	0.98
Phosphorus as (P_2O_5)	0.27	0.30	0.29
Sulfur as (SO_3)	0.13	0.25	0.20

TABLE XVIII

CLOVIS POINT BURN SLAG COMPOSITION

Mineral analysis (Wt. %)	Location 1	Location 2
Iron as Fe_2O_3	8.0	8.0
Calcium as CaO	19.0	18.0
Magnesium as MgO	5.0	6.0
Sodium as Na_2O	<3.0	<3.0
Potassium as K_2O	<1.0	<1.0
Silicon as SiO_2	46.0	47.0
Aluminum as Al_2O_3	18.0	18.0
Titanium as TiO_2	2.0	2.0
Phosphorus as P_2O_5	<1.0	1.0
Sulfur as SO_3	---	---

Data from Calgon Corporation

(Zecchini, 1986)

TABLE XIX

CLOVIS POINT-OKLAHOMA BURN SLAG COMPOSITION

Mineral analysis- (Wt %)	Wall	Wall	Bottom	Glassy	Crystalline
Iron as Fe_2O_3	6.0	5.0	7.0	7.0	7.0
Calcium as CaO	20.0	25.0	18.0	18.0	20.0
Magnesium as MgO	5.0	6.0	6.0	5.0	5.0
Sodium as Na_2O	4.0	<3.0	5.0	5.0	3.0
Potassium as K_2O	<4.0	<1.0	<1.0	<1.0	<1.0
Silicon as SiO_2	43.0	38.0	43.0	46.0	45.0
Aluminum as Al_2O_3	18.0	15.0	17.0	15.0	17.0
Titanium as TiO_2	1.0	2.0	1.0	1.0	1.0
Phosphorus as P_2O_5	1.0	2.0	1.0	1.0	1.0
Sulfur as SO_3	----	5.0	----	----	---

Data from Calgon Corporation

(Zecchini, 1986)

will transport some of the aerosols upward. These particles will be partly captured on the walls of the lower temperature zones. Therefore, in an economizer sample, other elements such as silicon and aluminum can also be found in significant amounts.

Secondary superheat tubes are located in the 1200 - 1400^{0} C region. In this temperature zone the model predicts a sulfur free deposit. The superheat tubes, presented in this model, are located between 95 - 165 ft high where a low sulfur and low phosphorus deposit is predicted which is similar to the plant data shown in Table XVII.

As for higher temperature zones, the slag samples (Tables XVIII and XIX) tend to have high aluminum and silicon contents and more modest amounts of magnesium and calcium than in the previous two zones. This is because the oxides condense in this temperature zone. Similar results can also be demonstrated by this model. Oxides such as Al_2O_3, SiO_2, MgO and CaO deposit at medium elevations and removed as bottom slag, as shown in Figures 11 to 13.

The slagging flux predicted by this model shows a higher deposit accumulation rate in the lower stages of the boiler than in the upper levels. A high slagging flux is also observed in the convective zone. This may become the major source of fouling in the convective zone. The slag and fouling formed on the walls of the boiler, fall down under their own weight and finally are removed from the boiler as the bottom ash.

CHAPTER V

CONCLUSION

1. A simple fire side deposits model is developed to predict the solid and vapor distributions inside a boiler.

2. The mineral matter undergoes thermal decomposition, vaporization and recondensation. The Al, Si, Ca and Mg oxides tend to remain as bottom ash and form slag in the hot stages. The P, S, Na and K compounds are condensed mostly on the convective zone and become the major sources of fouling. In the middle temperature stages, iron oxides appear to be the dominant compounds of ash deposits.

3. A higher deposit accumulation rate occurs in the lower stages of a boiler and constitute a major portion of the bottom ash. A high slagging flux is also calculated in the convective zone. This may cause fouling in closely spaced superheater or reheater tubes.

4. The stable compounds of mineral matter can be assigned by evaluating their chemical equilibrium constants. Sulfur compounds in the coal are rapidly decomposed and in colder stages react with alkali metals to form Na_2SO_4 or $CaSO_4$. These compounds tend to condense in the convective zone of the boiler.

5. The amount of each stable compound deposited at

various locations can be determined from the vapor pressure of that compound. The vapor pressures of some compounds could not be found from previous literature. A simple estimation technique is developed and used. The results are in general agreement with actual power plant data.

6. The adiabatic flame temperature of a coal is calculated using regular coal analysis and a few operational parameters. The heating value of a coal is a major factor that can change the flame temperature drastically.

7. The formation of fireside deposits in a furnace depends on the composition and association of mineral matter liberated from the coal. Deposition of specific mineral species depends on their thermal behavior and the local gas temperature. Consequently, the composition of the deposit may vary throughout the combustor depending on the local temperature.

CHAPTER VI

RECOMMENDATION

1. Mechanisms of deposit formation may include vapor condensation on walls, formation and growth of particles, particle capture and particle adhesion (Garner and Seapan, 1984). More work needs to be done to incorporate the particle growth, capture and adhension mechanisms into the model.

2. The ash deposition tendencies of the coal are determined by the operating conditions and time history, therefore more specific experiments should be performed to test this model. The test furnace built by Wang (1988) should be used to collect the experimental data.

3. Vaporization of other species of ash should be studied at high temperature.

4. More reliable thermodynamic properties of the ash compounds should be surveyed to give more precise quantitative results.

5. The chemical composition of mineral matter is controlled mainly by thermodynamics, while kinetic information regarding ash vaporization also needs to be considered, especially for a short residence time furnace.

6. The composition of fly ash and the rate of the fly

ash leaving the boiler do not agree completely with the plant data. Therefore, Particles deposition is another factor that needs to be considered.

7. Further modification of this model needs to be done, in order to explain the problem which was experienced at PSO's Oolagah power plant.

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APPENDIXES

APPENDIX A

LISTING OF FORTRAN PROGRAM

```
*
$nofloatcalls
$storage:2
*
*                                                    Lo, Jeng-Yeng
*                                                        1987-1988
*****************************************************************
*
*
* This program can predict the rate of deposition and the
* composition of deposits formed at different locations in
* a boiler. A multicell, lumped parameter approach was
* used, assuming that the cells are well mixed and
* deposition occurs only by condensation of the stable
* minerals on the boilers tubes.
*
* Basis for material balance calculation is 100 g coal.
* All calculation are done on this basis. At the end the
* number are scale-up for the actual coal consumption rate.
*
*
*****************************************************************
*                                                               *
*                                                               *
* NOMENCLATURE                                                  *
*                                                               *
*                                                               *
* A(I), B(I), C(I), D(I): coefficients of heat capacity         *
*     equation, I=1 to 7, refering to H2O, H2, N2, O2,          *
*     CO2, SO2, CO                                              *
* AA,BB,CC,DD: overall coefficients of heat capacity            *
*              equation of inlet gas                            *
* AAA,BBA,CCA,DDA: overall coefficients of heat capacity        *
*                  equation of outlet gas                       *
* AL: weight of Al (g)                                          *
* ALE: weight of solid Al element  in a zone (g)                *
* ALE1: weight of vapor Al element in a zone (g)                *
* AL2O3: weight of Al2O3 (g)                                    *
* AL2O3A: amount of total Al2O3 in a zone (gmol)                *
* AL2O3L: wt% of Al2O3 in ASTM ash analysis                     *
* AL2O3N: amount of solid Al2O3 in a zone (gmol)                *
* ALOX: Al in Al2O3 form for solid (g)                          *
* ALOX1: Al in Al2O3 form for vapor (g)                         *
* ALP: wt% of solid Al2O3 in a zone                             *
* ALP1: wt% of vapor Al2O3 in a zone                            *
* ASH: boiler ash (g)                                           *
* ASHC: unburned carbon in boiler ash (g)                       *
* ASHLIB: laboratory ash (g)                                    *
* CA: weight of Ca (g)                                          *
* CAE: weight of solid Ca element in a zone (g)                 *
* CAE1:weight of vapor Ca element in a zone (g)                 *
* CAO: weight of CaO (g)                                        *
```

```
* CAOA: amount of total CaO in a zone (gmol)                    *
* CAOL: wt% of CaO in ASTM ash analysis                         *
* CAON: amount of solid CaO in a zone (gmol)                    *
* CAOX: Ca in CaO form for solid (g)                            *
* CAOX1: Ca in CaO form for vapor (g)                           *
* CAP: wt% of solid CaO in a zone                               *
* CAP1: wt% of vapor CaO in a zone                              *
* CAPOA: amount of total Ca3(PO4)2 in a zone (gmol)             *
* CAPON: amount of solid Ca3(PO4)2 in a zone (gmol)             *
* CASO4A: amount of total CaSO4 in a zone (gmol)                *
* CASO4N: amount of solid CaSO4 in a zone (gmol)                *
* CB0,CB1: temperature profile regression line parameters       *
*          in convective zone                                   *
* COA: amount of CO after combustion (gmol)                     *
* COC: mol% of CO in the flue gas                               *
* CO2A: amount of CO2 after combustion (gmol)                   *
* CO2C: mol% of CO2 in the flue gas                             *
* CR: burned carbon (g)                                         *
* CR1: carbon content in coal (g)                               *
* CT1,CT2,CT3,CT4,CT5,CT6,CT7:convective zone temp. (K)         *
* DAIR: amount of dry air required in burning coal (gmol)       *
* ER: energy released in burning coal (cal)                     *
* FACTOR: scale-up factor to change from 100 g coal to          *
*         actual coal consumption rate                          *
* FC: fixed carbon wt% (from proximate analysis)                *
* FE: weight of Al (g)                                          *
* FEE: weight of solid Fe element in a zone (g)                 *
* FEE1: weight of vapor Fe element in a zone (g)                *
* FE2O3: weight of Fe2O3 (g)                                    *
* FE3O4: weight of Fe3O4 (g)                                    *
* FE2O3A: amount of total Fe2O3 in a zone (gmol)                *
* FE3O4A: amount of total Fe3O4 in a zone (gmol)                *
* FE2O3L: wt% of Fe2O3 in ASTM ash analysis                     *
* FE2O3N: amount of solid Fe2O3 in a zone (gmol)                *
* FE3O4N: amount of solid Fe3O4 in a zone (gmol)                *
* FEOX: Fe in Fe2O3 form for solid (g)                          *
* FEOX1: Fe in Fe2O3 form for vapor (g)                         *
* FEP: wt% of solid Fe2O3 in a zone                             *
* FEP1: wt% of vapor Fe2O3 in a zone                            *
* FLUX: slagging flux in a zone, defined as rate of             *
*       deposit formed per unit area (kg/m**2-hr)               *
* FUEL: fuel consumption rate (ton/hr)                          *
* H: furnace height in various zone (ft)                        *
* HAD: functional form of energy balance equation               *
* HADD: first derivative of energy balance eqn. function        *
* HAIR: enthalpy of inlet air (cal)                             *
* HASHI: enthalpy of inlet ash (cal)                            *
* HCOAL: enthalpy of inlet coal (cal)                           *
* HEIGHT: height of the boiler (ft)                             *
* HFC: enthalpy of fixed carbon (cal)                           *
* HH2O: enthalpy of moisture in inlet coal (cal)                *
* HIN: total enthalpy input (cal)                               *
* H2OA: amount of H2O after combustion (gmol)                   *
```

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* H2OC: mol% of H2O in the flue gas                                  *
* H2OO: amount of H2O in inlet air (gmol)                           *
* HVM: enthalpy of volatile matter (cal)                            *
* HVH: higher heating value (btu/lb)                                *
* HVLT: total lower heating value (btu/lb)                          *
* IGFACT: ignition factor to correct ash composition based*
*         on ASTM ash analysis                                      *
* K: weight of K (g)                                                *
* K2CO3A: amount of total K2CO3 in a zone (gmol)                    *
* K2CO3N: amount of solid K2CO3 in a zone (gmol)                    *
* KE: weight of solid K element in a zone (g)                       *
* KE1: weight of vapor K element in a zone (g)                      *
* K2O: weight of K2O (g)                                            *
* K2OL: wt% of K2O in ASTM ash analysis                             *
* KOX: K in K2O form for solid (g)                                  *
* KOX1: K in K2O form for vapor (g)                                 *
* KP: wt% of solid K2O in a zone                                    *
* KP1: wt% of vapor K2O in a zone                                   *
* LENGTH: length of the boiler (ft)                                 *
* MG: weight of Mg (g)                                              *
* MGE: weight of solid Mg element in a zone (g)                     *
* MGE1: weight of vapor Mg element in a zone (g)                    *
* MGO: weight of MgO (g)                                            *
* MGOA: amount of total MgO in a zone (gmol)                        *
* MGOL: wt% of MgO in ASTM ash analysis                             *
* MGON: amount of solid MgO in a zone (gmol)                        *
* MGOX: Mg in MgO form for solid (g)                                *
* MGOX1: Mg in MgO form for vapor (g)                               *
* MGP: wt% of solid MgO in a zone                                   *
  MGP1: wt% of vapor MgO in a zone                                  *
  MULLA: amount of total mullite in a zone (gmol)                   *
* MULLN: amount of solid mullite in a zone (gmol)                   *
* NA: weight of Na (g)                                              *
* NACLA: amount of total NaCl in a zone (gmol)                      *
* NACLN: amount of solid NaCl in a zone (gmol)                      *
* NAE: weight of solid Na element in a zone (g)                     *
* NAE1: weight of vapor Na element in a zone (g)                    *
* NA2OL: wt% of Na2O in ASTM ash analysis                           *
* NAOX: Na in Na2O form for solid (g)                               *
* NAOX1: Na in Na2O form for vapor (g)                              *
* NAP: wt% of solid Na2O in a zone                                  *
* NAP1: wt% of vapor Na2O in a zone                                 *
* NASOA: amount of total Na2SO4 in a zone (gmol)                    *
* NASON: amount of solid Na2SO4 in a zone (gmol)                    *
* O2A: amount of O2 after combustion (gmol)                         *
* O2C: mol% of O2 in the flue gas                                   *
* O2R: required oxygen for coal burned (gmol)                       *
* O2TH: theorectical oxygen for coal burned (gmol)                  *
* P: percent excess air                                             *
* PAL2O3: vapor pressure of Al2O3 (mm Hg)                           *
* PCAO: vapor pressure of CaO (mm Hg)                               *
* PCAPO: vapor pressure of Ca3(PO4)2 (mm Hg)                        *
* PCASO4: vapor pressure of CaSO4 (mm Hg)                           *
```

```
* PE: weight of solid P element in a zone (g)                    *
* PE1: weight of vapor P element in a zone (g)                   *
* PFE2O3: vapor pressure of Fe2O3 (mm Hg)                        *
* PFE3O4: vapor pressure of Fe3O4 (mm Hg)                        *
* PK2CO3: vapor pressure of K2CO3 (mm Hg)                        *
* PMGO: vapor pressure of MgO (mm Hg)                            *
* PMULL: vapor pressure of mullite (mm Hg)                       *
* PNACL: vapor pressure of NaCl (mm Hg)                          *
* PNASO: vapor pressure of Na2SO4 (mm Hg)                        *
* POX: P in P2O5 form for solid (g)                              *
* POX1: P in P2O5 form for vapor (g)                             *
* PP: wt% of P2O5 in a zone                                      *
* PROD: total flue gas (gmol)                                    *
* PSIO2: vapor pressure of SiO2 (mm Hg)                          *
* PTIO2: vapor pressure of TiO2 (mm Hg)                          *
* PTI2O3: vapor pressure of Ti2O3 (mm Hg)                        *
* Q: numerical tolerance in computation of flame temp (K)        *
* RATIO: correction factor,(flame temp/peak temp)                *
* RAL2O3: amount of accumulated solid Al2O3 (gmol)               *
* RCAO: amount of accumulated solid CaO (gmol)                   *
* RCAPO: amount of accumulated solid Ca3(PO4)2 (gmol)            *
* RCASO4: amount of accumulated solid CaSO4 (gmol)               *
* RFE2O3: amount of accumulated solid Fe2O3 (gmol)               *
* RFE3O4: amount of accumulated solid Fe3O4 (gmol)               *
* RK2CO3: amount of accumulated solid K2CO3 (gmol)               *
* RMGO: amount of accumulated solid MgO (gmol)                   *
* RMULL: amount of accumulated solid mullite (gmol)              *
* RNACL: amount of accumulated solid NaCl (gmol)                 *
* RNASO: amount of accumulated solid Na2SO4 (gmol)               *
* RSIO2: amount of accumulated solid SiO2 (gmol)                 *
* RT1,RT2,RT3,RT4,RT5,RT6: radiative zone temperature (K)        *
* RTIO2: amount of accumulated solid TiO2 (gmol)                 *
* RTI2O3: amount of accumulated solid Ti2O3 (gmol)               *
* RB0, RB1: temperature profile regression line parameters*
*           in radiative zone                                    *
* S1: weight of S (g)                                            *
* SE: weight of solid S element in a zone (g)                    *
* SE1: weight of vapor S element in a zone (g)                   *
* SENT: sentinel to devide radiative andconvective zone          *
* SI: weight of Si (g)                                           *
* SIE: weight of solid Si element in a zone (g)                  *
* SIE1: weight of vapor Si element in a zone (g)                 *
* SIO2: weight of SiO2 (g)                                       *
* SIO2A: amount of total SiO2 in a zone (gmol)                   *
* SIO2L: wt% of SiO2 in ASTM ash analysis                        *
* SIO2N: amount of solid SiO2 in a zone (gmol)                   *
* SIOX: Si in SiO2 form for solid (g)                            *
* SIOX1: Si in SiO2 form for vapor (g)                           *
* SIP: wt% of solid SiO2 in a zone                               *
* SIP1: wt% of vapor SiO2 in a zone                              *
* SLAGWT: amount of total deposits in a zone (g)                 *
* SOX: S in SO3 form for solid (g)                               *
* SOX1: S in SO3 form for vapor (g)                              *
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```
* SO2A: amount of SO2 after combustion (gmol)                    *
* SO2C: mol% of SO2 in the flue gas                              *
* SP: wt% of solid SO3 in a zone                                 *
* SP1: wt% of vapor S)3 in a zone                                *
* SUMOX: total solid oxides in a zone (g)                        *
* SUMOX1: total vapor oxides in a zone (g)                       *
* T1: coal inlet temperature (K)                                 *
* T2: preheated air temperature (K)                              *
* TA: assumed temperature in Newton method (K)                   *
* TFLAME: adiabatic flame temperature (C)                        *
* TK: temperature in a zone (K)                                  *
* TNEW: new temperature in Newton method (K)                     *
* TR: reference state temperature (K)                            *
* UNBURN: wt% of carbon trapped in the boiler ash                *
* VAL2O3: amount of vapor Al2O3 in a zone (gmol)                 *
* VCAO: amount of vapor CaO in a zone (gmol)                     *
* VCAPO: amount of vapor Ca3(PO4)2 in a zone (gmol)              *
* VCASO4: amount of vapor CaSO4 in a zone (gmol)                 *
* VFE2O3: amount of vapor Fe2O3 in a zone (gmol)                 *
* VFE3O4: amount of vapor Fe3O4 in a zone (gmol)                 *
* VK2CO3: amount of vapor K2CO3 in a zone (gmol)                 *
* VMGO: amount of vapor MgO in a zone (gmol)                     *
* VMULL: amount of vapor mullite in a zone (gmol)                *
* VNACL: amount of vapor NaCl in a zone (gmol)                   *
* VNASO: amount of vapor Na2SO4 in a zone (gmol)                 *
* VSIO2: amount of vapor SiO2 in a zone (gmol)                   *
* VTIO2: amount of vapor TiO2 in a zone (gmol)                   *
* VTI2O3: amount of vapor Ti2O3 in a zone (gmol)                 *
* VEL: gas velocity in a combustor (ft/sec)                      *
* VOLUME: flue gas volume (lit)                                  *
* W: mol fraction of water in the inlet air                      *
* W1: water content in the inlet air (lb H2O/lb air)             *
* WIDTH: width of the boiler (ft)                                *
* X: percent of unburned carbon converted into CO                *
* XSAl: amount of excess Al to assign compound                   *
* XSCA: amount of excess Ca to assign compound                   *
* XSNA: amount of excess Na to assign compound                   *
* XSS: amount of excess S to assign compound                     *
* XSSI: amount of excess Si to assign compound                   *
*****************************************************************
*
      IMPLICIT REAL (A-Z)
      REAL A(7),B(7),C(7),D(7)
*
      DATA A / 7.701,6.483,7.44,6.713,4.728,5.697,7.373 /
      DATA B / 4.595E-4,2.215E-3,-0.324E-2,-0.879E-6,
     + 1.754E-2,1.6E-2,-0.307E-2 /
      DATA C / 2.521E-6,-3.298E-6,6.4E-6,4.17E-6,
     + -1.338E-5, -1.185E-5,6.662E-6 /
      DATA D / -0.859E-9,1.826E-9,-2.79E-9,-2.544E-9,
     + 4.097E-9,3.172E-9,-3.037E-9 /
*
      OPEN (6,FILE='COAL.OUT',STATUS='NEW')
```

```
*
*      READ INPUT DATA FROM KEYBOARD OR ANY DEFAULT DEVICE
*      ENTERING COAL ANALYSIS
       WRITE(*,*)'BASIS 100 GRAMS COAL SAMPLE '
       WRITE(*,*)'ENTER ULTIMATE ANALYSIS
      + (%)...H2O,C,H,N,S,O,ASH ?'
       READ(*,*)H2O,CR1,H,N,SUL,O,ASHLAB
       WRITE(*,*)'PROXIMATE ANALYSIS
      + (%)...FIXED C, VOLATILE MATTER ?'
       READ(*,*)FC,VM
       WRITE(*,*)'COAL HIGH HEATING VALUE ? '
       READ(*,*)HVH
*
*      ENTERING ASTM ASH ANALYSIS
       WRITE(*,*)' ASTM ASH ANALYSIS
      + (WT%)...SIO2,AL2O3,TIO2,FE2O3,CAO'
       READ(*,*)SIO2L,AL2O3L,TIO2L,FE2O3L,CAOL
       WRITE(*,*)'
      + ....MGO,NA2O,K2O,P2O5,SO3     '
       READ(*,*)MGOL,NA2OL,K2OL,P2O5L,SO3L
*
       WRITE(*,*)'EXCESS AIR(%) ,WATER CONTENT IN AIR (LB
      + H2O/LB AIR)'
       READ(*,*) P, W1
       WRITE(*,*)'% CARBON UNBURNED IN ASH,
      + % CARBON CONVERTED INTO CO '
       READ(*,*)UNBURN,X
       WRITE(*,*)'COAL INLET TEMPERATURE &
      + PREHEATED AIR TEMPERATURE(C)'
       READ(*,*) TT1,TT2
*
       WRITE(*,*)'ENTER WIDTH, LENGTH, HEIGHT OF BOILER (FT)'
       READ(*,*)WIDTH, LENGTH,HEIGHT
       WRITE(*,*)'ENTER FUEL CONSUMPTION RATE (TON/HR) '
       READ(*,*)FUEL
* END OF INPUT
*****************************************************************

       TR    = 298.0
       T1    = TT1+273.0
       T2    = TT2+273.0
       ASHC  = UNBURN*ASHLAB/(100.0-UNBURN)
       ASH   = ASHLAB+ASHC
       CR    = CR1-ASHC
*
*      CONVERT ASTM ASH WT% INTO WEIGHT IN GRAMS
       IGFACT  = 100.0/(SIO2L+AL2O3L+TIO2L+FE2O3L+CAOL
      +  +MGOL+NA2OL+K2OL+P2O5L+SO3L)
       SIO2    = SIO2L*ASHLAB/100.0*IGFACT
       AL2O3   = AL2O3L*ASHLAB/100.0*IGFACT
       TIO2    = TIO2L*ASHLAB/100.0*IGFACT
       FE2O3   = FE2O3L*ASHLAB/100.0*IGFACT
       CAO     = CAOL*ASHLAB/100.0*IGFACT
```

```
      MGO      = MGOL*ASHLAB/100.0*IGFACT
      NA2O     = NA2OL*ASHLAB/100.0*IGFACT
      K2O      = K2OL*ASHLAB/100.0*IGFACT
      P2O5     = P2O5L*ASHLAB/100.0*IGFACT
      SO3      = SO3L*ASHLAB/100.0*IGFACT
*
*     CALCULATE COAL ENTHALPY INPUT === HCOAL
*     HCOAL    : HFC + HASHI + HVM + HH2OC
*
      HFC  = FC*(0.145*(T1-TR)+(2.35E-4)*(T1**2-TR**2)-
     + (0.8767E-7)*(T1**3-TR**3)+(1.3125E-11)*(T1**4-TR**4))
      HASHI= ASH*(0.18*(T1-TR)+(3.89E-5)*(T1**2-TR**2))
      HVM  = VM*(0.4128*(T1-TR)+(2.195E-4)*(T1**2-TR**2))
      HH2OC= H2O*1.0*(T1-TR)
      HCOAL= HFC+HASHI+HVM+HH2OC
*
*     CALCULATE AIR ENTHALPY INPUT === HAIR
*
      O2TH = (CR/12.0)+(H/2.0)*0.5+(SUL/32.0)-(O/32.0)
      O2R  = O2TH*(1.0+P/100.0)
      NR   = O2R*79.0/21.0
      DAIR = NR+O2R
      W    = (W1/18.0)/(W1/18.0+1.0/28.96)
      H2OO = (W*DAIR)/(1.0-W)
*
*     CALCULATE HEAT CAPACITY COEFFICIENT OF INLET AIR
*
      AA   = A(1)*H2OO+A(3)*NR+A(4)*O2R
      BB   = B(1)*H2OO+B(3)*NR+B(4)*O2R
      CC   = C(1)*H2OO+C(3)*NR+C(4)*O2R
      DD   = D(1)*H2OO+D(3)*NR+D(4)*O2R
      HAIR = AA*(T2-TR)+BB*(T2**2-TR**2)/2.0+CC*(T2**3-
     + TR**3)/3.0+DD*(T2**4-TR**4)/4.0
*
*     FLUE GAS COMPOSITION CALCULATION
*
      H2OA = H2OO+(H2O/18.0)+(H/2.0)
      CO2A = CR*(100.0-X)/1200.0
      COA  = CR*X/1200.0
      SO2A = SUL/32.0
      NA   = NR+N/28.0
      O2A  = O2R-CO2A-(0.5*COA)-(H*0.25)-SO2A+(O/32.0)
*
*     VOL % OF FLUE GAS
*
      PROD = H2OA+COA+CO2A+SO2A+NA+O2A
      H2OC = H2OA*100.0/PROD
      CO2C = CO2A*100.0/PROD
      COC  = COA*100.0/PROD
      SO2C = SO2A*100.0/PROD
      NC   = NA*100.0/PROD
      O2C  = O2A*100.0/PROD
*
```

```
*      COAL HEATING VALUE AND ENERGY RELEASE
*      HVLT      : HVH MIMUS HEAT OF VAPORZATION OF THE WATER
*
       HVLT = HVH*0.002204*100.0*252.0-H/2.0*18.0*0.002204
      +        *1050.0*252.0
       ER   = HVLT-HVH*0.002204*252.0*ASHC
*
* TOTAL INPUT ENTHALPY (HIN):ENTHALPY INPUT OF COAL(HCAOL)
*                          + ENTHALPY INPUT OF AIR  (HAIR)
*                          + COAL ENERGY RELEASE    (ER)
*
       HIN  = HCOAL+HAIR+ER
*
* CALCULATE AFTER COMBUSTION FLUE GAS HEAT CAPACITY CONSTANT
*
       AAA  = A(5)*CO2A+A(1)*H2OA+A(3)*NA+
      + A(4)*O2A+SO2A*A(6)+A(7)*COA
       BBA  = B(5)*CO2A+B(1)*H2OA+B(3)*NA+
      + B(4)*O2A+SO2A*B(6)+B(7)*COA
       CCA  = C(5)*CO2A+C(1)*H2OA+C(3)*NA+
      +  C(4)*O2A+SO2A*C(6)+C(7)*COA
       DDA  = D(5)*CO2A+D(1)*H2OA+D(3)*NA+
      + D(4)*O2A+SO2A*D(6)+D(7)*COA
*
* HCOAL+HAIR+HEAT GENERATED (HVLT) = HASH+HFLUEGAS
*
* NEWTON-RAPHSON METHOD TO SOLVE FLAME TEMPERATURE
* TA IS INITIAL TEST FLAME TEMPERATURE IN DEGREE K
       TA   = 2200.0
* HAD:ENTHALPY CHANGE AFTER REACTIONS (FUNCTION OF TEMP )
* HADD IS THE FIRST DERIVATIVE OF HAD(T)
* ABS(Q) IS THE TOLERANCE
  200  HAD  = ((AAA+(ASH*0.18))*(TA-TR))+((BBA+(7.78E-5)
      + *ASH)*(TA**2-TR**2)/2.0)+(CCA*(TA**3-TR**3)/3.0)
      + +(DDA*(TA**4-TR**4)/4.0)-HIN
       HADD = (AAA+(ASH*0.18))+((BBA+(7.78E-5)*ASH)*TA)
      + +(CCA*(TA**2))+(DDA*(TA**3))
       TNEW = TA-HAD/HADD
       Q    = TA-TNEW
       IF(ABS(Q) .LE. 0.001) GO TO 300
       TA   = TNEW
       GO TO 200
  300  TK   = TA
       TFLAME= TK-273.0
* END OF ADIABATIC FLAME TEMPERATURE
*************************************************************

* ASSIGN POSSIBLE STABLE COMPOUND DURING COMBUSTION
*      POSSIBLE MAJOR SULFATES  IN COAL DEPOSITS :
*               NA2SO4,CASO4
*      POSSIBLE MAJOR OXIDES    IN COAL DEPOSITS :
*               CAO,MGO,FE2O3,FE3O4,AL2O3,TIO2,TI2O3,SIO2
*      POSSIBLE MAJOR PHOSPHATES IN COAL DEPOSITS:
```

```
*               CA3(PO4)2
*      OTHER POSSIBLE COMPOUND IN COAL DEPOSITS:
*               NACL, AL6SI2O13, K2CO3
*
       S1   = SO3*(32.0/(32.0+48.0))
       CA   = CAO*(40.08/(40.08+16.0))
       NA   = NA2O*(23.0*2.0/(46.0+16.0))
       K    = K2O*(39.1*2.0/(39.1*2.0+16.0))
       TI   = TIO2*(47.9/79.9)
       AL   = AL2O3*(2*26.98/101.96)
       SI   = SIO2*(28.09/60.08)
       FE   = FE2O3*(2*55.85/159.69)
       PH   = P2O5*(2*30.97/(2*30.97+80.0))
*
*      CONVERT AL INTO MULLITE(AL6SI2O13), AL2O3
*      CONVERT SI INTO MULLITE(AL6SI2O13), SIO2
       ALMOLE = AL/26.98
       SIMOLE = SI/28.09
       AL6    = ALMOLE/6
       SI2    = SIMOLE/2
       IF (AL6 .GE. SI2) THEN
       MULL   = SI*426.05/(2*28.09)
       XSAL     = AL - MULL*6*26.98/426.05
       AL2O3    = XSAL*(2*26.98+48)/(2*26.98)
       ELSE
       MULL   = AL*426.05/(6*26.98)
       XSSI     = SI - MULL*2*28.09/426.05
       SIO2     = XSSI*60.08/28.09
       ENDIF
*
*      CONVERT FE WEIGHT INTO FE2O3, FE3O4 ( 2 : 3 )
       FE2O3    = FE*0.4*159.69/(2.0*55.85)
       FE3O4    = FE*0.6*231.54/(3.0*55.85)
*
*      CONVERT TI WEIGHT INTO TIO2, TI2O3 ( 1 : 2 )
       TIO2     = TI*(1.0/3.0)*(79.9/47.9)
       TI2O3    = TI*(2.0/3.0)*143.8/(47.9*2.0)
*
*      CONVERT PO4 INTO CA3(PO4)2
       CAPO     = PH*310.18/(30.97*2)
       XSCA     = CA - CAPO*3*40.08/310.18
       CA       = XSCA
*
* IF CL GREATER OR EQUAL THAN 0.6 ,THEN CL SERVE AS NACL
* IF CL LESS THAN 0.6 ,THEN CL CAN BE IGNORED
* CONVERT NA INTO NA2SO4
* CONVERT CA INTO CASO4, CAO
*
       IF (CL .GE. 0.6) THEN
       NACL   = CL*((23.0+35.45)/35.45)
       XSNA   = NA-NACL*(23.0/(35.45+23.0))
       ELSE
       NACL   = 0.0
```

```
      XSNA    = NA
      ENDIF
*
* EXCESS NA AS NA2SO4
      NA2SO4 = XSNA*(23.0*2.0+32.0+64.0)/(23.0*2.0)
      XSS    = S1-NA2SO4*32.0/(23.0*2.0+32.0+64.0)
*
* IF EXCESS S GREATER THAN 0.0 ,EXCESS S AS CASO4
* THEN IF EXCESS CA GREATER THAN 0.0 ,EXCESS CA AS CAO
* IF EXCESS CA LESS THAN 0.0,RECALCULATE CASO4 AND NA2SO4
      IF (XSS .GT. 0.0) THEN
      CASO4  = XSS*(40.0+32.0+64.0)/32.0
      XSCA   = CA-CASO4*40.0/(40.0+32.0+64.0)
      CAO    = XSCA*(40.0+16.0)/40.0
* IF EXCESS CA <0.0 ,CA AS CASO4 AND EXCESS S AS NA2SO4
       IF (XSCA .LT. 0.0) THEN
       CASO4  = CA*(40.0+32.0+64.0)/40.0
       XSS    = S1-CASO4*32.0/(40.0+32.0+64.0)
       NA2SO4 = XSNA*(46.0+32.0+64.0)/46.0
       XSS    = XSS-NA2SO4*(46.0+32.0+64.0)/46.0
       ENDIF
      ENDIF
*
*     CONVERT K2O INTO K2CO3
      K2CO3  = K*138.2/(2*39.1)
*
*     WEIGHT OF TOTAL MINERAL
      TOWT= MULL+AL2O3+SIO2+FE3O4+FE2O3+NACL+
     +  NA2SO4+CAPO+CASO4+CAO+TIO2+TI2O3+K2CO3+MGO
* END OF POSSIBL STABLE COMPOUND ASSIGNED
*****************************************************************

*     LIST THE OUTPUT RESULTS
      WRITE(6,*)'*******************************************'
      WRITE(6,*)'CALCULATION OF MINERAL MATTER DISTRIBUTION'
      WRITE(6,*)'           IN A COAL FIRED BOILER          '
      WRITE(6,*)'*******************************************'
      WRITE(6,*)' '
      WRITE(6,*)'INPUT DATA:'
      WRITE(6,*)' '
      WRITE(6,*)'              ULTIMATE ANLYSIS        WT%  '
      WRITE(6,*)'=========================================='
      WRITE(6,*)'  H2O    C     H     N    S     O    ASH  '
      WRITE(6,50)H2O,CR1,H,N,SUL,O,ASHLAB
   50 FORMAT(F7.2,F7.2,F7.2,F7.2,F7.2,F7.2,F7.2,/)
*
      WRITE(6,*)'         PROXIMATE ANALYSIS       WT%      '
      WRITE(6,*)'=========================================='
      WRITE(6,*)' FIXED C  VOLATILE MATTER  H2O   ASH     '
      WRITE(6,60)FC,VM,H2O,ASHLAB
   60 FORMAT(F10.2,F14.2,F10.2,F7.2,/)
*
      WRITE(6,*)'    ASTM ASH ANALYSIS          WT %       '
```

```
      WRITE(6,*)'=========================================='
      WRITE(6,*)'   SIO2     AL2O3     TIO2    FE2O3    CAO   '
      WRITE(6,70)SIO2L,AL2O3L,TIO2L,FE2O3L,CAOL
   70 FORMAT(F8.2,F8.2,F8.2,1X,F8.2,2X,F8.2)
      WRITE(6,*)'   MGO      NA2O       K2O    P2O5      SO3   '
      WRITE(6,80)MGOL,NA2OL,K2OL,P2O5L,SO3L
   80 FORMAT(F8.2,F8.2,F8.2,1X,F8.2,2X,F8.2,/)
*
      WRITE(6,*)'                INPUT FUEL DATA               '
      WRITE(6,*)'=========================================='
      WRITE(6,*)'COAL T(C) AIR T(C) EX AIR %  H2O IN AIR %'
      WRITE(6,90)TT1,TT2,P,W
   90 FORMAT(F10.2,F10.2,F12.2,F12.2,/)
*
      WRITE(6,11)HVH
   11 FORMAT('HIGHER HEATING VALUE= ', F8.0,' BTU/LB',/)
      WRITE(6,12)UNBURN
   12 FORMAT('UNBURNED CARBON IN ASH= ',F4.2,' %',/)
      WRITE(6,14)X
   14 FORMAT('CARBON CONVERTED TO CO= ',F4.2,' %',/)
      WRITE(6,15)FUEL
   15 FORMAT('FUEL CONSUMPTION RATE= ',F6.0,' TON/HR',/)
      WRITE(6,*)'DIMENSION OF BOILER:  (FT)'
      WRITE(6,16)WIDTH,LENGTH,HEIGHT
   16 FORMAT('WIDTH= ',F4.0,'LENGTH= ',F4.0,'HEIGHT= ',
     + F4.0,/)
*
      WRITE(6,*)'OUTPUT DATA:'
      WRITE(6,*)' '
      WRITE(6,*)'          FLUE GAS COMPOSITION       VOL%'
      WRITE(6,*)'=========================================='
      WRITE(6,*)'   H2O     CO2    CO     SO2     N2      O2 '
      WRITE(6,100)H2OC,CO2C,COC,SO2C,NC,O2C
  100 FORMAT(F8.2,F8.2,F8.2,F8.2,F8.2,F8.2,/)
*
      WRITE(6,17)PROD
   17 FORMAT('FLUE GAS (FOR 100 g COAL)= ',F6.3,'GMOL')
      WRITE(6,*)' '
      WRITE(6,18)ASH
   18 FORMAT('BOILER ASH= ',F6.4,' GRAMS',/)
      WRITE(6,110)TFLAME
  110 FORMAT('ADIABATIC FLAME TEMPERATURE= ',F6.0, '(C)',/)
*
*     CONVERT WEIGHTS OF MINERAL INTO MOLES OF MINERAL
      MULLA    = MULL/426.05
      AL2O3A   = AL2O3/101.96
      SIO2A    = SIO2/60.08
      FE2O3A   = FE2O3/159.69
      FE3O4A   = FE3O4/231.54
      NASOA    = NA2SO4/142.04
      NACLA    = NACL/(23+35.45)
      CAPOA    = CAPO/310.18
      CASO4A   = CASO4/136.14
```

```
      CAOA     = CAO/56.08
      TIO2A    = TIO2/79.9
      TI2O3A   = TI2O3/143.8
      MGOA     = MGO/40.3
      K2CO3A   = K2CO3/138.2
*
      RMULL    = 0.0
      RAL2O3   = 0.0
      RSIO2    = 0.0
      RFE2O3   = 0.0
      RFE3O4   = 0.0
      RNASO    = 0.0
      RNACL    = 0.0
      RCAPO    = 0.0
      RCASO4   = 0.0
      RCAO     = 0.0
      RTIO2    = 0.0
      RTI2O3   = 0.0
      RMGO     = 0.0
      RK2CO3   = 0.0
* SCALE-UP FACTOR TO CONVERT 100g COAL TO ACTUAL BURNING
* RATE
      FACTOR = FUEL*1000.0*1000.0/100.0
* CURVE FITTING TEMPERATURE PROFILES
* USING DEFAULT PROFILE OR INPUT TEMPERATURE PROFILE
      WRITE(*,*)'IS TEMPERATURE PROFILE AVAILABLE?
     + YES=1, NO=0'
      READ(*,*)COUNT
      IF (COUNT .GT. 0) THEN
      WRITE(*,*)'ENTER RADIATION ZONE TEMPERATURE AT  '
      WRITE(*,*)'FLAME,30FT,60FT,90FT,120FT,150FT,165FT (K)'
      READ(*,*)RT1,RT2,RT3,RT4,RT5,RT6,RT7
*     RADIATION ZONE
      RATIO = TK/RT1
      SY=(RT1+RT2+RT3+RT4+RT5+RT6+RT7)*RATIO
      SX=0.0+30.0+60.0+90.0+120.0+150.0+165.0
      SXX=0+30**2+60**2+90**2+120**2+150**2+165**2
      SXY=(RT1*0.0+RT2*30.0+RT3*60.0+RT4*90.0+RT5*120.0
     +     +RT6*150.0+RT6*165.0)*RATIO
* B1= (N*SUM(X*Y)-SUMX*SUMY)/(N*SUM(X**2)-SUMX**2)
* B0= (SUMY-B1*SUMX)/N
      RB1     = (7*SXY-SX*SY)/(7.0*SXX-SX**2)
      RB0     = (SY-RB1*SX)/7.0
      WRITE(*,*)'RADIATION ZONE T PROFILE : '
      WRITE(*,*)' T = ( ',RB1,' ) * H + ( ',RB0,' ) '
*     TK      = RB1*H+RB0
*
      WRITE(*,*)'ENTER CONVECTION ZONE TEMPERATURE AT '
      WRITE(*,*)'165FT,180FT,195FT,210FT,225FT,240FT (K)'
      READ(*,*)CT1,CT2,CT3,CT4,CT5,CT6
*     CONVECTION ZONE
      SY=(CT1+CT2+CT3+CT4+CT5+CT6)*RATIO
      SX=165.0+180.0+195.0+210.0+225.0+240.0
```

```
      SXX=165.0**2+180.0**2+195.0**2+210.0**2
     +    +225.0**2+240.0**2
      SXY=(CT1*165.0+CT2*180.0+CT3*195.0+CT4*210.0
     +    +CT5*225.0+CT6*240.0)*RATIO
      CB1    = (6*SXY-SX*SY)/(6.0*SXX-SX**2)
      CB0    = (SY-CB1*SX)/6.0
      WRITE(*,*)'CONVECTION ZONE T PROFILE : '
      WRITE(*,*)' T = ( ',CB1,' ) * H + ( ',CB0,' ) '
*     TK     = CB1*H+CB0
*
      ELSE
* CURVE FITTING DEFAULT PROFILE
* RADIATION ZONE
* RESIDENCE TIME: 0.067  0.5  1.0  1.5  2.0  2.5  2.75 SEC
* TEMPERATURE   : 2348   2246 2107 1968 1921 1848 1764  K
* ASSUME AVERAGE VELOCITY IS 60.0 FT/SEC
      VEL    = 60.0
      RATIO  = TK/2348.0
      SY=(2348.0+2246.0+2107.0+1968.0+1921.0+1848.0+1764.0)
     +    *RATIO
      SX=(0.067+0.5+1.0+1.5+2.0+2.5+2.75)*VEL
      SXX=(VEL*0.067)**2+(VEL*0.5)**2+VEL**2+(VEL*1.5)
     +   **2+(VEL*2.0)**2+(VEL*2.5)**2+(VEL*2.75)**2
      SXY=(2348.0*0.067+2246.0*0.5+2107.0*1.0+1968.0*1.5
     + +1921.0*2.+1848.0*2.5+1764.0*2.75)*VEL*RATIO
      RB1=(7*SXY-SX*SY)/(7.0*SXX-SX**2)
      RB0=(SY-RB1*SX)/7.0
      WRITE(*,*)'RADIATION ZONE T PROFILE : '
      WRITE(*,*)' T = ( ',RB1,' ) * H + ( ',RB0,' ) '
*     TK     = RB1*H+RB0
*
* CONVECTION ZONE
* RESIDENCE TIME: 2.75  3.0  3.25  3.5  3.75  4.0 SEC
* TEMPERATURE   : 1764  1551 1227  996  811   672  K
      SY=(1764.0+1551.0+1227.0+996.0+811.0+672.0)*RATIO
      SX=(2.75+3.0+3.25+3.5+3.75+4.0)*VEL
      SXX=(2.75*VEL)**2+(3.0*VEL)**2+(3.25*VEL)**2+
     + (3.5*VEL)**2 +(3.75*VEL)**2+(4.0*VEL)**2
      SXY=(1764.0*2.75+1551.0*3.0+1227.0*3.25+996.0*3.5
     + +811.0*3.75+4.0*672.0)*VEL*RATIO
      CB1=(6*SXY-SX*SY)/(6.0*SXX-SX**2)
      CB0=(SY-CB1*SX)/6.0
      WRITE(*,*)'CONVECTION ZONE T PROFILE : '
      WRITE(*,*)' T = ( ',CB1,' ) * H + ( ',CB0,' ) '
*     TK     = CB1*H+CB0
      END IF
* END OF TEMPERATURE PROFILE
*************************************************************

* THE DISTRIBUTION OF MINERAL MATTERS AT DIFFERENT LOCATIONS
* DEVIDED A COMBUSTOR INTO ZONES AND EACH WITH 10 FEET IN
* HEIGHT
* MINERAL DISTRIBUTION IN RADIATIVE ZONE
```

```
      SENT    = 165.0
      H       = -5.0
  210 IF (H .LT. SENT) THEN
      H       = H+10.0
      TK      = RB1*H+RB0
      WRITE(6,87)H,TK
   87 FORMAT('Height: ',F4.0,' ft, Temperature: ',F5.0,' K')
      CALL RESIDUAL(RMULL,RAL2O3,RSIO2,RFE2O3,RFE3O4,RNASO,
     +      RNACL,RCAPO,RCASO4,RCAO,RTIO2,RTI2O3,RMGO,RK2CO3,
     +      MULLA,AL2O3A,SIO2A,FE2O3A,FE3O4A,NASOA,NACLA,
     +      CAPOA,CASO4A,CAOA,TIO2A,TI2O3A,MGOA,K2CO3A,
     +      TK,PROD,VOLUME,WIDTH,LENGTH,FACTOR)
      GO TO 210
      ELSE
      GO TO 220
      END IF
* MINERAL DISTRIBUTION IN CONVECTIVE ZONE
  220 H       = 165.0
      SENT    = HEIGHT
  230 IF  (H .LT. SENT) THEN
      H       = H+10.0
      TK      = CB1*H+CB0
      WRITE(6,97)H,TK
   97 FORMAT('Height: ',F4.0,' ft, Temperature: ',F5.0,' K')
      CALL RESIDUAL(RMULL,RAL2O3,RSIO2,RFE2O3,RFE3O4,RNASO,
     +RNACL,RCAPO,RCASO4,RCAO,RTIO2,RTI2O3,RMGO,RK2CO3,
     +MULLA,AL2O3A,SIO2A,FE2O3A,FE3O4A,NASOA,NACLA,
     +CAPOA,CASO4A,CAOA,TIO2A,TI2O3A,MGOA,K2CO3A,
     +TK,PROD,VOLUME,WIDTH,LENGTH,FACTOR)
      GO TO 230
      END IF

      STOP
      END
*
* SUBROUTINE TO CALCULATE THE AMOUNT OF VAPOR AND SOLID IN
* EACH ZONE
*
      SUBROUTINE RESIDUAL(RMULL,RAL2O3,RSIO2,RFE2O3,
     +RFE3O4,RNASO,RNACL,RCAPO,RCASO4,RCAO,RTIO2,RTI2O3,
     +RMGO,RK2CO3,MULLA,AL2O3A,SIO2A,FE2O3A,FE3O4A,NASOA,
     +NACLA,CAPOA,CASO4A,CAOA,TIO2A,TI2O3A,MGOA,K2CO3A,
     +TK,PROD,VOLUME,WIDTH,LENGTH,FACTOR)
      IMPLICIT REAL (A-Z)
*
* SINCE AT HIGH TEMPERATURE LOW PRESSURE ,THEREFORE,
* FOLLOW THE IDEAL GAS LAW TO CALCULATE FLUE GAS VOLUME
* ASSUMPTION:
* 1.PARTIAL PRESSURES OF MINERAL VAPORS ARE THE SAME AS
* VAPOR PRESSURE OF MINERAL MATTERS
* 2.TOTAL PRESSURE IS 760 MMHG
* GAS CONSTANT (R) = 62.36(L*MMHG)/(GMOLE*K)
* VAPOR PRESSURE EQUATIONS OF MINERAL MATTERS
```

```
      R         = 62.36
      VOLUME    = (PROD*R*TK)/760.0
      PMULL=(EXP(13.08-39552.3468/TK))*760.0
      PAL2O3=(10**(13.42-27320.0/TK))*(7.500617*(1.0E-3))
      PSIO2=(10**(13.43-26428.38/TK))
      PFE2O3=(EXP(14.0925-38536.8397/TK))*760.0
      PFE3O4=(10**(14.24-22780.0/TK))*(7.500617*(1.0E-3))
      PNASO=(10**(5.37-11062.0/TK))*760.0
      PNACL=10**((-11495/TK)-3.526*ALOG10(TK)+20.929)
      PCAPO=(EXP(10.5677-31734.7734/TK))*760.0
      PCASO4=(EXP(10.5677-28247.4348/TK))*760.0
      PCAO=(10**(12.85-28020.0/TK))*(7.500617*(1.0E-3))
      PTIO2=(10**(14.37-30060.0/TK))*(7.500617*(1.0E-3))
      PTI2O3=(10**(31.68-64700/TK-1.26*(1.0E-3)/TK))
     +   *(7.500617*(1.0E-3))
      PMGO=(10**(12.37-26100.0/TK))*(7.500617*(1.0E-3))
      PK2CO3=(10**(5.39-(12700.0/TK)))*760.0
*
* CALCULATE MAXIMUM MOLES OF MINERAL MATTERS IN VAPOR PHASE
*
      VMULL     = PMULL*VOLUME/(62.36*TK)
      VAL2O3    = PAL2O3*VOLUME/(62.36*TK)
      VSIO2     = PSIO2*VOLUME/(62.36*TK)
      VFE2O3    = PFE2O3*VOLUME/(62.36*TK)
      VFE3O4    = PFE3O4*VOLUME/(62.36*TK)
      VCAPO     = PCAPO*VOLUME/(62.36*TK)
      VCASO4    = PCASO4*VOLUME/(62.36*TK)
      VCAO      = PCAO*VOLUME/(62.36*TK)
      VNASO     = PNASO*VOLUME/(62.36*TK)
      VNACL     = PNACL*VOLUME/(62.36*TK)
      VTIO2     = PTIO2*VOLUME/(62.36*TK)
      VTI2O3    = PTI2O3*VOLUME/(62.36*TK)
      VMGO      = PMGO*VOLUME/(62.36*TK)
      VK2CO3    = PK2CO3*VOLUME/(62.36*TK)
*
* COMPARED ASH BETWEEN AVAILABLE AND MAXIMMUM POSSIBLE
*
      MULLN     = MULLA-VMULL
      AL2O3N    = AL2O3A-VAL2O3
      SIO2N     = SIO2A-VSIO2
      FE2O3N    = FE2O3A-VFE2O3
      FE3O4N    = FE3O4A-VFE3O4
      CAPON     = CAPOA-VCAPO
      CASO4N    = CASO4A-VCASO4
      CAON      = CAOA-VCAO
      NASON     = NASOA-VNASO
      NACLN     = NACLA-VNACL
      TIO2N     = TIO2A-VTIO2
      TI2O3N    = TI2O3A-VTI2O3
      MGON      = MGOA-VMGO
      K2CO3N    = K2CO3A-VK2CO3
*
      IF (MULLN .LT. 0.0) THEN
```

```
      MULLN  = 0.0
      MULLA  = MULLA-MULLN
      ELSE
      RMULL  = MULLN+RMULL
      MULLA  = VMULL
      WMULL  = MULLN*426.05
      END IF
*
      IF (AL2O3N .LT. 0.0) THEN
      AL2O3N     = 0.0
      AL2O3A     = AL2O3A-AL2O3N
      ELSE
      RAL2O3     = AL2O3N+RAL2O3
      AL2O3A     = VAL2O3
      WAL2O3     = AL2O3N*101.96
      END IF
*
      IF (SIO2N .LT. 0.0) THEN
      SIO2N      = 0.0
      SIO2A      = SIO2A-SIO2N
      ELSE
      RSIO2      = SIO2N+RSIO2
      SIO2A      = VSIO2
      WSIO2      = SIO2N*60.08
      END IF
*
      IF (FE2O3N .LT. 0.0) THEN
      FE2O3N    = 0.0
      FE2O3A    = FE2O3A-FE2O3N
      ELSE
      RFE2O3    = RFE2O3+FE2O3N
      FE2O3A    = VFE2O3
      WFE2O3    = FE2O3N*159.69
      END IF
*
      IF (FE3O4N .LT. 0.0) THEN
      FE3O4N    = 0.0
      FE3O4A    = FE3O4A-FE3O4N
      ELSE
      RFE3O4    = RFE3O4+FE3O4N
      FE3O4A    = VFE3O4
      WFE3O4    = FE3O4N*231.54
      END IF
*
      IF (CAPON .LT. 0.0) THEN
      CAPON = 0.0
      CAPOA = CAPOA-CAPON
      ELSE
      RCAPO = RCAPO+CAPON
      CAPOA = VCAPO
      WCAPO = CAPON*310.18
      END IF
*
```

```
      IF (CASO4N .LT. 0.0) THEN
      CASO4N    = 0.0
      CASO4A    = CASO4A-CASO4N
      ELSE
      RCASO4    = RCASO4+CASO4N
      CASO4A    = VCASO4
      WCASO4    = CASO4N*136.14
      END IF
*
      IF (CAON .LT. 0.0) THEN
      CAON      = 0.0
      CAOA      = CAOA-CAON
      ELSE
      RCAO      = CAON+RCAO
      CAOA      = VCAO
      WCAO      = CAON*56.08
      END IF
*
      IF (NASON .LT. 0.0) THEN
      NASON  = 0.0
      NASOA  = NASOA-NASON
      ELSE
      RNASO  = NASON+RNASO
      NASOA  = VNASO
      WNASO  = NASON*142.04
      END IF
*
      IF (NACLN .LT. 0.0) THEN
      NACLN     = 0.0
      NACLA     = NACLA-NACLN
      ELSE
      RNACL     = RNACL+NACLN
      NACLA     = VNACL
      WNACL     = NACLN*58.45
      END IF
*
      IF (TIO2N .LT. 0.0) THEN
      TIO2N      = 0.0
      TIO2A      = TIO2A-TIO2N
      ELSE
      RTIO2      = TIO2N+RTIO2
      TIO2A      = VTIO2
      WTIO2      = TIO2N*79.9
      END IF
*
      IF (TI2O3N .LT. 0.0) THEN
      TI2O3N     = 0.0
      TI2O3A     = TI2O3A-TI2O3N
      ELSE
      RTI2O3     = TI2O3N+RTI2O3
      TI2O3A     = VTI2O3
      WTI2O3     = TI2O3N*143.8
      END IF
```

```
*
      IF (MGON .LT. 0.0) THEN
      MGON      = 0.0
      MGOA      = MGOA-MGON
      ELSE
      RMGO      = MGON+RMGO
      MGOA      = VMGO
      WMGO      = MGON*40.3
      END IF
*
      IF (K2CO3N .LT. 0.0) THEN
      K2CO3N    = 0.0
      K2CO3A    = K2CO3A-K2CO3N
      ELSE
      RK2CO3    = K2CO3N+RK2CO3
      K2CO3A    = VK2CO3
      WK2CO3    = K2CO3N*138.2
      END IF
*
* WEIGHT OF SLAG PRODUCED BY BURNING 100g COAL IN A ZONE
      SLAGWT = WMULL+WAL2O3+WSIO2+WFE2O3+WFE3O4+WCAPO
     +       +WCASO4+WCAO+WNASO+WNACL+WTIO2+WTI2O3
     +       +WMGO+WK2CO3
* BOILER SLAG BUILD UP RATE: FLUX (KG/M**2-HR)
      AREA = 2*(WIDTH+LENGTH)*10*0.092903
      FLUX = (SLAGWT*FACTOR/(1000.0*AREA))
      WRITE(6,89)SLAGWT
   89 FORMAT('SLAG = ',F8.5,'GRAMS (FOR 100 GRAMS COAL)')
      WRITE(6,99)FLUX
   99 FORMAT('SLAGGING FLUX = ',F8.3,' KG/M**2-HR ')
* CONVERT ASH DEPOSITION INTO ASTM ASH ANALYSIS
*     CONVERT DEPOSIT INTO ELEMENT
      FEE=FE2O3N*2*55.85/159.69+FE3O4N*3*55.85/231.54
      CAE=CAON*40.08/56.08+CAPON*40.08/310+CASO4N*40.08
     +    /136.14
      MGE=MGON*24.31/40.3
      NAE=NASON*46/142.04+NACLN*23/58.45
      KE =K2CO3N*2*39.1/138.2
      SIE=SIO2N*28.09/60.08+MULLN*2*28.09/426.05
      ALE=AL2O3N*2*26.98/101.96+MULLN*6*26.98/426.05
      TIE=TIO2N*47.9/79.9+TI2O3N*2*47.9/143.8
      PE =CAPON*2*30.97/310.18
      SE =CASO4N*32.06/136.14+NASON*32.06/142.04
*     CONVERT ELEMENT INTO OXIDE
      FEOX=FEE*159.69/55.85/2
      CAOX=CAE*56.08/40.08
      MGOX=MGE*40.3/24.31
      NAOX=NAE*62/23/2
      KOX =KE*94.2/39.1/2
      SIOX=SIE*60.08/28.09
      ALOX=ALE*101.96/26.98/2
      TIOX=TIE*79.9/47.9
      POX =PE*141.94/30.97/2
```

```
      SOX =SE*80.06/32.06
*     CONVERT INTO ASTM ASH ANALYSIS
      SUMOX=FEOX+CAOX+MGOX+NAOX+KOX+SIOX+ALOX+TIOX+POX+SOX
      FEP=FEOX*100.0/SUMOX
      CAP=CAOX*100.0/SUMOX
      MGP=MGOX*100.0/SUMOX
      NAP=NAOX*100.0/SUMOX
      KP =KOX*100.0/SUMOX
      SIP=SIOX*100.0/SUMOX
      ALP=ALOX*100.0/SUMOX
      TIP=TIOX*100.0/SUMOX
      PP =POX*100.0/SUMOX
      SP =SOX*100.0/SUMOX
      WRITE(6,*)'DISTRIBUTION OF SOLID MINERAL MATTER (WT%)'
      WRITE(6,*)'Fe as    Ca as  Mg as   Na as  K  as  '
      WRITE(6,*)'Fe2O3    CaO    MgO     Na2O   K2O    '
      WRITE(6,88)FEP,CAP,MGP,NAP,KP
   88 FORMAT(5F7.2)
      WRITE(6,*)'Si as    Al as  Ti as   P as   S  as  '
      WRITE(6,*)'SiO2     Al2O3  TiO2    P2O5   SO3    '
      WRITE(6,98)SIP,ALP,TIP,PP,SP
   98 FORMAT(5F7.2,/)
* CONVERT VAPOR INTO ASTM ASH ANALYSIS
*     CONVERT VAPOR INTO ELEMENT
      FEE1=VFE2O3*2*55.85/159.69+VFE3O4*3*55.85/231.54
      CAE1=VCAO*40.08/56.08+VCAPO*40.08/310+VCASO4*40.08
     + /136.14
      MGE1=VMGO*24.31/40.3
      NAE1=VNASO*46/142.04+VNACL*23/58.45
      KE1 =VK2CO3*2*39.1/138.2
      SIE1=VSIO2*28.09/60.08+VMULL*2*28.09/426.05
      ALE1=VAL2O3*2*26.98/101.96+VMULL*6*26.98/426.05
      TIE1=VTIO2*47.9/79.9+VTI2O3*2*47.9/143.8
      PE1 =VCAPO*2*30.97/310.18
      SE1 =VCASO4*32.06/136.14+VNASO*32.06/142.04
*     CONVERT ELEMENT INTO OXIDE
      FEOX1=FEE1*159.69/55.85/2
      CAOX1=CAE1*56.08/40.08
      MGOX1=MGE1*40.3/24.31
      NAOX1=NAE1*62/23/2
      KOX1 =KE1*94.2/39.1/2
      SIOX1=SIE1*60.08/28.09
      ALOX1=ALE1*101.96/26.98/2
      TIOX1=TIE1*79.9/47.9
      POX1 =PE1*141.94/30.97/2
      SOX1 =SE1*80.06/32.06
*     CONVERT INTO ASTM ASH ANALYSIS
      SUMOX1=FEOX1+CAOX1+MGOX1+NAOX1+KOX1+SIOX1
     +       +ALOX1+TIOX1+POX1+SOX1
      FEP1=FEOX1*100.0/SUMOX1
      CAP1=CAOX1*100.0/SUMOX1
      MGP1=MGOX1*100.0/SUMOX1
      NAP1=NAOX1*100.0/SUMOX1
```

```
      KP1 =KOX1*100.0/SUMOX1
      SIP1=SIOX1*100.0/SUMOX1
      ALP1=ALOX1*100.0/SUMOX1
      TIP1=TIOX1*100.0/SUMOX1
      PP1 =POX1*100.0/SUMOX1
      SP1 =SOX1*100.0/SUMOX1
      WRITE(6,*)'DISTRIBUTION OF VAPOR DISTRIBUTION (WT%)'
      WRITE(6,*)'Fe as     Ca as  Mg as   Na as  K  as  '
      WRITE(6,*)'Fe2O3     CaO    MgO     Na2O   K2O    '
      WRITE(6,188)FEP1,CAP1,MGP1,NAP1,KP1
  188 FORMAT(5F7.2)
      WRITE(6,*)'Si as     Al as  Ti as   P as   S  as  '
      WRITE(6,*)'SiO2      Al2O3  TiO2    P2O5   SO3    '
      WRITE(6,198)SIP1,ALP1,TIP1,PP1,SP1
  198 FORMAT(5F7.2,/)
      RETURN
      END
```

APPENDIX B

INSTRUCTIONS FOR PROGRAM INPUTS AND OUTPUTS

PROGRAM INPUT

```
C> COAL
BASIS 100 GRAMS COAL SAMPLE
ENTER ULTIMATE ANALYSIS (%)...H2O,C,H,N,S,ASH ?
-
[Input ultimate analysis from coal analysis]

PROXIMATE ANALYSIS (%)...FIXED C, VOLATILE MATTER ?
-
[Input fixed carbon and volatile matter wt % from coal
analysis]

COAL HIGH HEATING VALUE ?
-
[Read from coal analysis or calculate from Dulong's formular
(btu/lb)]

ASTM ASH ANALYSIS (WT%)...SIO2,AL2O3,TIO2,FE2O3,CAO
-
                         ...MGO,NA2O,K2O,P2O5,SO3
-
[Input ASTM ash analysis from coal analysis]

EXCESS AIR(%), WATER CONTENT IN AIR (LB H2O/LB AIR)
-
[Input excess air %, usually between 10 to 30. Water content
read from psychrometric chart]

% CARBON UNBURNED IN ASH, % CARBON CONVERTED INTO CO
-
[Input carbon trappedin the ash, usually between 5 to 15.
Input carbon converted into CO]

COAL INLET TEMPERATURE & PREHEATED AIR TEMPERATURE (C)
-
[Input coal inlet temperature and preheated air temperature]

ENTER WIDTH, LENGTH, HEIGHT OF BOILER (FT)
-
[Input the dimension of the boiler]

ENTER FUEL CONSUMPTION RATE (TON/HR)
-
```

IS TEMPERATURE PROFILE AVAILABLE? YES=1, NO=0
-
[Input "0" then default temperature profile is chosen, program starts to execute. Input "1" then continue to key in the input value]

ENTER RADIATION ZONE TEMPERATURE AT
FLAME, 30FT, 60FT, 90FT, 120FT, 150FT, 165FT (K)
-
[Input combustor temperatures starting from bottom]

ENTER CONVECTION ZONE TEMPERATURE AT
165FT, 180Ft, 195FT, 210FT, 225Ft, 240FT (K)
-
[Input combustor temperature of these location. If temperature is hard to measure, interpolation may be used]

PROGRAM OUTPUT

The output data will be saved in a automatically created file named COAL.OUT. Two types of output files were developed. A more complete output file can list all the input parameters, flue gas composition, adiabatic flame temperature, the rate of deposition and the compositon of deposits formed in every 10 feet interval within the furnace. A sample output is shown on the next page. Another type of output file is to generate data file directly. This data file shows the amount of solid and vapor in every 10 feet interval and can be directly transferred into LOTUS 123 to generate graphs of the vapor and solid distributions which are shown in chapter IV.

```
*******************************************
CALCULATION OF MINERAL MATTER DISTRIBUTION
          IN A COAL FIRED BOILER
*******************************************

 INPUT DATA:

              ULTIMATE ANLYSIS              WT%
 ================================================
   H2O      C       H       N      S       O      ASH
 25.44   48.43    3.96     .69     .64   14.03    6.81

               PROXIMATE ANALYSIS           WT%
 ================================================
 FIXED C    VOLATILE MATTER    H2O    ASH
    31.20          36.55      25.44   6.81

          ASTM ASH ANALYSIS              WT %
 ================================================
    SIO2     AL2O3     TIO2    FE2O3     CAO
   46.38    13.81     1.15     7.15      14.22
    MGO      NA2O      K2O     P2O5      SO3
    3.15      .68     1.37     1.11       6.05

               INPUT FUEL DATA
 ================================================
 COAL T (C) AIR T  (C)  EXCESS AIR %  WATER IN AIR %
     30.00     300.00        15.00          .03

HIGHER HEATING VALUE=    8863. BTU/LB

UNBURNED CARBON IN ASH= 5.00 %

CARBON CONVERTED TO CO= 2.00 %

FUEL CONSUMPTION RATE=   300. TON/HR

 DIMENSION OF BOILER:  (FT)
WIDTH=  50.LENGTH=  50.HEIGHT= 220.

 OUTPUT DATA:

          FLUE GAS COMPOSITION          VOL%
 ================================================
     H2O      CO2      CO       SO2      N2       O2
   14.59    13.64     .28      .07    68.89     2.52

FLUE GAS (FOR 100 g COAL)= 28.781GMOL

BOILER ASH= 7.1684 GRAMS

ADIABATIC FLAME TEMPERATURE=  1709. (C)
```

Height: 5. ft, Temperature: 1958. K
SLAG = 2.93253GRAMS (FOR 100 GRAMS COAL)
SLAGGING FLUX = 87.976 KG/M**2-HR
DISTRIBUTION OF SOLID MINERAL MATTER (WT%)

Fe as Fe2O3	Ca as CaO	Mg as MgO	Na as Na2O	K as K2O
.00	26.83	12.60	.00	.00

Si as SiO2	Al as Al2O3	Ti as TiO2	P as P2O5	S as SO3
37.27	21.76	1.54	.00	.00

DISTRIBUTION OF VAPOR DISTRIBUTION (WT%)

Fe as Fe2O3	Ca as CaO	Mg as MgO	Na as Na2O	K as K2O
.30	.36	.00	85.16	2.11

Si as SiO2	Al as Al2O3	Ti as TiO2	P as P2O5	S as SO3
.05	.02	.00	.06	11.93

Height: 225. ft, Temperature: 701. K
SLAG = .00004GRAMS (FOR 100 GRAMS COAL)
SLAGGING FLUX = .001 KG/M**2-HR
DISTRIBUTION OF SOLID MINERAL MATTER (WT%)

Fe as Fe2O3	Ca as CaO	Mg as MgO	Na as Na2O	K as K2O
.00	.24	.00	43.07	.74

Si as SiO2	Al as Al2O3	Ti as TiO2	P as P2O5	S as SO3
.00	.00	.00	.00	55.95

DISTRIBUTION OF VAPOR DISTRIBUTION (WT%)

Fe as Fe2O3	Ca as CaO	Mg as MgO	Na as Na2O	K as K2O
.00	.00	.00	99.01	.01

Si as SiO2	Al as Al2O3	Ti as TiO2	P as P2O5	S as SO3
.00	.00	.00	.00	.99

VITA

Jeng-Yeng Lo

Candidate for the Degree of

Master of Science

Thesis: A SIMPLE MODEL FOR SIMULATION OF THE FATE OF MINERAL MATTERS IN A COAL FIRED BOILER

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Taipei, Taiwan, June 25, 1954, son of Shew-Lin Jen and Thi-Jen Lo.

Education: Graduated from Chen-Kuo High School, Taipei, Taiwan, in June, 1973; received the Bachelor of Science Degree in Chemical Engineering from Cheng-Kung University in June, 1977; completed the requirements for the Master of Science degree in Chemical Engineering at Oklahoma State University in July, 1988.

Professional Experience: Employed by Chinese Petroleum Corporation, Kaohsiung, Taiwan, as a chemical engineer, November 1977 to August 1986; Research assistant of Chemical Engineering Department, Oklahoma State University, September 1986 to May 1988.